INFORMATION TO USERS

This was produced from a copy of a document sent to us for microfilming. While the most advanced technological means to photograph and reproduce this document have been used, the quality is heavily dependent upon the quality of the material submitted.

The following explanation of techniques is provided to help you understand markings or notations which may appear on this reproduction.

1. The sign or “target” for pages apparently lacking from the document photographed is “Missing Page(s)”. If it was possible to obtain the missing page(s) or section, they are spliced into the film along with adjacent pages. This may have necessitated cutting through an image and duplicating adjacent pages to assure you of complete continuity.

2. When an image on the film is obliterated with a round black mark it is an indication that the film inspector noticed either blurred copy because of movement during exposure, or duplicate copy. Unless we meant to delete copyrighted materials that should not have been filmed, you will find a good image of the page in the adjacent frame.

3. When a map, drawing or chart, etc., is part of the material being photographed the photographer has followed a definite method in “sectioning” the material. It is customary to begin filming at the upper left hand corner of a large sheet and to continue from left to right in equal sections with small overlaps. If necessary, sectioning is continued again—beginning below the first row and continuing on until complete.

4. For any illustrations that cannot be reproduced satisfactorily by xerography, photographic prints can be purchased at additional cost and tipped into your xerographic copy. Requests can be made to our Dissertations Customer Services Department.

5. Some pages in any document may have indistinct print. In all cases we have filmed the best available copy.
PLEASE NOTE:

In all cases this material has been filmed in the best possible way from the available copy. Problems encountered with this document have been identified here with a check mark ‾.

1. Glossy photographs □
2. Colored illustrations □
3. Photographs with dark background □
4. Illustrations are poor copy □
5. Print shows through as there is text on both sides of page □
6. Indistinct, broken or small print on several pages □
7. Tightly bound copy with print lost in spine □
8. Computer printout pages with indistinct print □
9. Page(s) □ lacking when material received, and not available from school or author
10. Page(s) □ seem to be missing in numbering only as text follows
11. Poor carbon copy □
12. Not original copy, several pages with blurred type □
13. Appendix pages are poor copy □
14. Original copy with light type □
15. Curling and wrinkled pages □
16. Other □

University
Microfilms
International
THE ELECTROMAGNETIC PROPERTIES
OF SMALLMETAL PARTICLE MIXTURES

DISSERTATION

Presented in Partial Fulfillment of the Requirements
for the Degree Doctor of Philosophy in the Graduate
School of The Ohio State University

By
Richard Lee Henry, B.A., M.S.

* * * * *

The Ohio State University
1980

Reading Committee:
Prof. David B. Tanner
Prof. James C. Garland
Prof. David Stroud

Approved By

Adviser
Department of Physics
ACKNOWLEDGMENTS

I would like to thank my adviser, Dr. David B. Tanner for his enthusiasm and guidance; Roy S. Tucker for his help with the smoke evaporations, Ottis E. Campbell for his instruction in machine shop operations, Jeffrey H. Franklin for operating the scanning electron microscope, the staff of the Physics Department shop for making many of the Lamellar grating interferometer parts, and the staff of the Instruction and Research Computer Center for their help with the software. I would also like to thank Marlene M. Pease for typing this dissertation.
VITA

June 16, 1950 . . . . Born - Cleveland, Ohio

1971 . . . . . . . B.A., University of Northern Colorado

1973-1974 . . . . Teaching Assistant, Physics Depart­
ment, Cleveland State University, Cleveland, Ohio

1974 . . . . . . . M.S. in Physics, Cleveland State University

1974-1980 . . . . Teaching Associate, Physics Depart­
ment, The Ohio State University, Columbus, Ohio

PUBLICATIONS


PRESENTATIONS


# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACKNOWLEDGMENTS</td>
<td>ii</td>
</tr>
<tr>
<td>VITA</td>
<td>iii</td>
</tr>
<tr>
<td>LIST OF TABLES</td>
<td>viii</td>
</tr>
<tr>
<td>LIST OF FIGURES</td>
<td>ix</td>
</tr>
<tr>
<td>LIST OF PLATES</td>
<td>xv</td>
</tr>
<tr>
<td>Chapter</td>
<td></td>
</tr>
<tr>
<td>I. INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>II. THEORY</td>
<td>5</td>
</tr>
<tr>
<td>A. Polarization of a Sphere</td>
<td>6</td>
</tr>
<tr>
<td>1) Simple Expressions</td>
<td>8</td>
</tr>
<tr>
<td>2) Polarizabilities from Mie Theory</td>
<td>9</td>
</tr>
<tr>
<td>a) Mie's solution for a sphere in an electromagnetic field</td>
<td>9</td>
</tr>
<tr>
<td>b) Electric polarizability from the Mie fields</td>
<td>23</td>
</tr>
<tr>
<td>c) Magnetic polarizability from the Mie fields</td>
<td>24</td>
</tr>
<tr>
<td>3) Comparison of the Mie polarizabilities with the simple expressions</td>
<td>26</td>
</tr>
<tr>
<td>a) Electric case</td>
<td>27</td>
</tr>
<tr>
<td>b) Magnetic case</td>
<td>33</td>
</tr>
<tr>
<td>B. Effective Medium Theories</td>
<td>40</td>
</tr>
<tr>
<td>1) Maxwell Garnett Approximation</td>
<td>40</td>
</tr>
</tbody>
</table>
a) Electric case ........................ 41
b) Magnetic case ........................ 49

2) Effective Medium Approximation ......... 51
3) Low Concentration Limit ................ 54

C. Models for Powder Samples ................. 55
   1) Solid Metal Particle Models ........... 57
   2) Clustered Particle Models .............. 59
   3) Effects of the Particle and Cluster Size Distributions .......... 64
      a) Volume Averaged Particle Diameter .. 64
      b) Summation of Contributions of Different Diameters .......... 65

III. EXPERIMENTAL PROCEDURE ......................... 71
   A. Fourier Transform Spectroscopy ............ 72
      1) Basic Mathematical Formulation .......... 73
         a) Finite maximum path difference ..... 74
         b) Discretely sampled interferograms .. 76
         c) Errors in the location of zero path difference ............... 77
      2) Typical Interferometers ................. 78
         a) Lamellar grating interferometer .... 78
         b) Michelson Interferometer ............. 82
   B. Construction, Peripheral Equipment and Operation of the OSU Lamellar Grating Interferometer ................ 83
      1) Construction of the OSU Lamellar Grating Interferometer .......... 85
      2) Cryostat ................................ 88
### C. Sample Preparation and Characterization

1) Smoke evaporation .......................... 101  
2) Mixture preparation ...................... 104  
3) Determination of volume filling fractions ....................... 109  
4) Determination of particle and cluster sizes .................. 111  
   a) Scanning electron microscopy and x-ray mapping .......... 111  
   b) SEM sample mounting .................... 115  
   c) Determination of the particle and cluster diameter distributions ...... 116  

### D. Hydrogenation of Palladium

1) The palladium hydride system .......... 124  
2) Hydrogenation technique ............... 125  

### IV. ANALYSIS

A. Corrections for Systematic Errors ........ 133  
   1) Interference pattern ..................... 134  
   2) Sample holder ............................ 134  
   3) The alumina powder ..................... 135  
   4) Detector nonlinearities .................. 141  
   5) Reflection from the sample surfaces ... 144  
   6) The metal volume fraction ............... 148
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>B. Fit of Theory to Experiment</td>
<td>149</td>
</tr>
<tr>
<td>V. DISCUSSION</td>
<td>186</td>
</tr>
<tr>
<td>Appendices</td>
<td></td>
</tr>
<tr>
<td>A. HARMONICALLY VARYING ELECTROMAGNETIC FIELDS</td>
<td>190</td>
</tr>
<tr>
<td>B. COMPUTER PROGRAMS</td>
<td>196</td>
</tr>
<tr>
<td>1) TOP</td>
<td>197</td>
</tr>
<tr>
<td>2) OUTGFILE</td>
<td>199</td>
</tr>
<tr>
<td>3) DEDUCE</td>
<td>221</td>
</tr>
<tr>
<td>4) FIT</td>
<td>233</td>
</tr>
<tr>
<td>5) Plotting Subroutines</td>
<td>286</td>
</tr>
<tr>
<td>LIST OF REFERENCES</td>
<td>295</td>
</tr>
</tbody>
</table>
# LIST OF TABLES

<table>
<thead>
<tr>
<th>Table</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Mie coefficients for 70 cm(^{-1}) radiation incident on a palladium sphere immersed in vacuum</td>
<td>17</td>
</tr>
<tr>
<td>2. Special functions used in Mie theory</td>
<td>18</td>
</tr>
<tr>
<td>3. Small argument approximations for (j_n(z)) and (h_n^{(1)}(z))</td>
<td>19</td>
</tr>
<tr>
<td>4. Typical instrument settings</td>
<td>96</td>
</tr>
<tr>
<td>5. Details of evaporations</td>
<td>105</td>
</tr>
<tr>
<td>6. Densities of components of mixtures</td>
<td>110</td>
</tr>
<tr>
<td>7. X-Ray emission lines used for SEM X-Ray mapping</td>
<td>114</td>
</tr>
<tr>
<td>8. Particle and cluster sizes</td>
<td>123</td>
</tr>
<tr>
<td>9. Concentration of hydrogen in the palladium samples</td>
<td>130</td>
</tr>
<tr>
<td>10. Results of parabolic fitting procedure</td>
<td>150</td>
</tr>
<tr>
<td>11. Results of the least-square fitting of the theory to the experimental data</td>
<td>173</td>
</tr>
</tbody>
</table>
# LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Coordinate axes used in Mie's solution for a sphere in an electromagnetic field</td>
<td>11</td>
</tr>
<tr>
<td>2</td>
<td>The real part of the electric polarizability versus sphere diameter size at 70 cm(^{-1}) for palladium spheres</td>
<td>28</td>
</tr>
<tr>
<td>3</td>
<td>The real part of the electric polarizability versus wavenumber for 1 (\mu m) diameter palladium spheres</td>
<td>29</td>
</tr>
<tr>
<td>4</td>
<td>The imaginary part of the electric polarizability versus sphere diameter at 70 cm(^{-1}) for palladium spheres</td>
<td>30</td>
</tr>
<tr>
<td>5</td>
<td>Enlarged View of the imaginary part of the electric polarizability versus sphere diameter at 70 cm(^{-1}) for palladium spheres</td>
<td>31</td>
</tr>
<tr>
<td>6</td>
<td>The imaginary part of the electric polarizability versus wavenumber for 1 (\mu m) diameter palladium spheres</td>
<td>32</td>
</tr>
<tr>
<td>7</td>
<td>The real part of the magnetic polarizability versus sphere diameter at 70 cm(^{-1}) for palladium spheres</td>
<td>34</td>
</tr>
<tr>
<td>8</td>
<td>The real part of the magnetic polarizability versus wavenumber for 1 (\mu m) diameter palladium spheres</td>
<td>35</td>
</tr>
<tr>
<td>9</td>
<td>The imaginary part of the magnetic polarizability versus sphere diameter at 70 cm(^{-1}) for palladium spheres</td>
<td>37</td>
</tr>
<tr>
<td>10</td>
<td>Enlarged view of the imaginary part of the magnetic polarizability versus sphere diameter at 70 cm(^{-1}) for palladium spheres</td>
<td>38</td>
</tr>
<tr>
<td>11</td>
<td>The imaginary part of the magnetic polarizability versus wavenumber for 1 (\mu m) diameter palladium spheres</td>
<td>39</td>
</tr>
<tr>
<td>No.</td>
<td>Description</td>
<td>Page</td>
</tr>
<tr>
<td>-----</td>
<td>-------------</td>
<td>------</td>
</tr>
<tr>
<td>12.</td>
<td>Composite material between the capacitor plates</td>
<td>44</td>
</tr>
<tr>
<td>13.</td>
<td>Composite material after an effective medium was substitutes for most of the inclusions and the host material</td>
<td>45</td>
</tr>
<tr>
<td>14.</td>
<td>Normalized absorption coefficient versus wavenumber for 0.14 μm diameter palladium spheres using the solid particle models and 50 times the room temperature, bulk conductivity</td>
<td>58</td>
</tr>
<tr>
<td>15.</td>
<td>Normalized absorption coefficient versus wavenumber for 13 μm diameter palladium clusters with a metal filling fraction within the clusters of 0.34 and a metal conductivity of 50 times the room temperature, bulk value</td>
<td>60</td>
</tr>
<tr>
<td>16.</td>
<td>Normalized absorption coefficient versus wavenumber for 13 μm diameter palladium clusters with a metal filling fraction within the clusters of 0.16 and a metal conductivity of 50 times the room temperature, bulk value</td>
<td>63</td>
</tr>
<tr>
<td>17.</td>
<td>Normalized absorption coefficient versus wavenumber for solid palladium spheres with 50 times the room temperature, bulk conductivity and diameters which follow a log-normal distribution</td>
<td>67</td>
</tr>
<tr>
<td>18.</td>
<td>Normalized absorption coefficient versus wavenumber for clustered palladium spheres with a metal conductivity 50 times the room temperature, bulk value. The clusters have a metal filling fraction of 0.34 and diameters which follow a log-normal distribution</td>
<td>69</td>
</tr>
<tr>
<td>19.</td>
<td>Light reflecting from a lamellar grating</td>
<td>79</td>
</tr>
<tr>
<td>20.</td>
<td>Optical plan of the OSU lamellar grating interferometer</td>
<td>81</td>
</tr>
<tr>
<td>21.</td>
<td>Optical plan of the OSU Michelson interferometer</td>
<td>84</td>
</tr>
<tr>
<td>22.</td>
<td>The cryostat</td>
<td>89</td>
</tr>
</tbody>
</table>
23. Evaporator used to make smoke evaporated particles ............................... 102
24. Absorption coefficient of high density polyethylene ............................................. 106
25. Polyethylene sample container ............................................................... 108
26. Cluster diameter distribution for sample 173-3 on a linear scale ............................................. 119
27. Cluster diameter distribution for sample 173-3 on a logarithmic scale ........................... 120
28. Reference chamber for determining the hydrogen concentration with the palladium samples ............................................. 127
29. Absorption coefficient of sample holder after soaking in hydrogen .................. 136
30. Absorption coefficient (normalized by dividing by the alumina filling fraction) of alumina C ............................................. 138
31. Absorption coefficient (normalized by dividing by the alumina filling fraction) of Alumina B ............................................. 139
32. Absorption coefficient (normalized by dividing by the alumina filling fraction) of alumina 0.3 ............................................. 140
33. Normalized, corrected absorption coefficient for sample 147-2, Pd (0.036), versus wavenumber. The fitted parabolic line is also shown ............................................. 151
34. Normalized, corrected absorption coefficient for sample 174-4, Pd(0.036), versus wavenumber. The fitted parabolic line is also shown ............................................. 152
35. Normalized, corrected absorption coefficient for sample 174-4 with hydrogen, Pd \(H_0^{0.036}\) versus wavenumber. The fitted parabolic line is also shown ............................................. 153
36. Normalized, corrected absorption coefficient for sample 149-2, Pd(0.062), versus wavenumber. The fitted parabolic line is also shown ........................................154

37. Normalized, corrected absorption coefficient for sample 174-5, Pd(0.062), versus wavenumber. The fitted parabolic line is also shown ........................................155

38. Normalized, corrected absorption coefficient for sample 162-3, Pd(0.14), versus wavenumber. The fitted parabolic line is also shown ........................................156

39. Normalized, corrected absorption coefficient for sample 162-4, Pd(0.14), versus wavenumber. The fitted parabolic line is also shown ........................................157

40. Normalized, corrected absorption coefficient for sample 173-2, Pd(0.14), versus wavenumber. The fitted parabolic line is also shown ........................................158

41. Normalized, corrected absorption coefficient for sample 173-2 with hydrogen, Pd H_{0.8}(0.14), versus wavenumber. The fitted parabolic line is also shown ............159

42. Normalized, corrected absorption coefficient for sample 156-5, Pd(0.57), versus wavenumber. The fitted parabolic line is also shown ........................................160

43. Normalized, corrected absorption coefficient for sample 173-4, Pd(0.57), versus wavenumber. The fitted parabolic line is also shown ........................................161

44. Normalized, corrected absorption coefficient for sample 173-4 with hydrogen, Pd H_{0.8}(0.57), versus wavenumber. The fitted parabolic line is also shown ............162

45. Normalized, corrected absorption coefficient for sample 156-3, Pd(1.9), versus wavenumber. The fitted parabolic line is also shown ........................................163
46. Normalized, corrected absorption coefficient for sample 173-3, Pd(1.9), versus wavenumber. The fitted parabolic line is also shown .......................... 164

47. Normalized, corrected absorption coefficient for sample 173-3 with hydrogen, Pd H_{0.8}(1.9) versus wavenumber. The fitted parabolic line is also shown .......... 165

48. Normalized, corrected absorption coefficient for sample 162-5, (AG-Pd)(0.33), versus wavenumber. The fitted parabolic line is also shown .......................... 166

49. Normalized, corrected absorption coefficient for sample 173-5, (AG-Pd)(0.33), versus wavenumber. The fitted parabolic line is also shown .......................... 167

50. Normalized, corrected absorption coefficient for sample 174-3, Au(0.19), versus wavenumber. The fitted parabolic line is also shown .......................... 168

51. Normalized, corrected absorption coefficient for sample 174-2, Au(1.3), versus wavenumber. The fitted parabolic line is also shown .......................... 169

52. Normalized, corrected absorption coefficient for sample 144-3, oxidized gold, versus wavenumber. The fitted parabolic line is also shown .......................... 170

53. Normalized, corrected absorption coefficient for sample 144-4, oxidized palladium, versus wavenumber. The fitted parabolic line is also shown .......................... 171

54. Normalized, corrected absorption coefficient for sample 173-2, Pd(0.14), versus wavenumber. The fitted theoretical line is also shown .......................... 175

55. Normalized, corrected absorption coefficient for sample 173-2 with hydrogen, Pd H_{0.8}(0.14), versus wavenumber. The fitted theoretical line is also shown .......... 176
56. Normalized, corrected absorption coefficient for sample 173-4, Pd(0.57), versus wavenumber. The fitted theoretical line is also shown .................................. 177

57. Normalized, corrected absorption coefficient for sample 173-4 with hydrogen, Pd H₀.₈(0.57), versus wavenumber. The fitted theoretical line is also shown ........ 178

58. Normalized, corrected absorption coefficient for sample 173-3, Pd(1.9), versus wavenumber. The fitted theoretical line is also shown .................................. 179

59. Normalized, corrected absorption coefficient for sample 173-3 with hydrogen, Pd H₀.₈(1.9), versus wavenumber. The fitted theoretical line is also shown ........ 180

60. Normalized, corrected absorption coefficient for sample 173-5, (AG-Pd)(0.33), versus wavenumber. The fitted theoretical line is also shown ............................. 181

61. Normalized, corrected absorption coefficient for sample 174-2, Au(1.3), versus wavenumber. The fitted theoretical line is also shown .................................. 182

62. Theoretical, normalized absorption coefficient versus the relaxation time of the metal for sample 173-3 ......................... 188
# LIST OF PLATES

<table>
<thead>
<tr>
<th>Plate</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>I.</td>
<td>Scanning electron micrograph of the mixture used in sample 173-3 (500X)</td>
<td>117</td>
</tr>
<tr>
<td>II.</td>
<td>Palladium x-ray map of the region shown in Plate I</td>
<td>117</td>
</tr>
<tr>
<td>III.</td>
<td>A typical inclusion that was found in the mixture used in sample 173-3 (5000X)</td>
<td>118</td>
</tr>
<tr>
<td>IV.</td>
<td>Palladium x-ray map of the region shown in Plate III</td>
<td>118</td>
</tr>
</tbody>
</table>
CHAPTER I

Introduction

The properties of a randomly inhomogeneous material made up of a mixture of several homogeneous materials are different from the properties of the component materials. This dissertation will be concerned with the average far-infrared absorption coefficient of such a mixture. The inhomogeneous materials studied here were binary mixtures consisting of a metal powder mixed with an insulating powder. In the course of this study, both theoretical predictions and experimental measurements were performed. To attempt to separate the influence of the geometric arrangement of the different components from the properties of the components themselves, measurements were made on several samples before and after changing the chemical make-up of one of the components. For the samples investigated, the theoretical calculations are in good agreement with the experimental results.
Historically, metal powder-insulator mixtures have been studied by many workers. The earliest optical measurements were made by Harris and Beasley\textsuperscript{1} in the near infrared to near ultraviolet spectral region. Further experimental measurements in this spectral region have been performed by McKenzie\textsuperscript{2} and Granqvist and Hunderi.\textsuperscript{3} Far infrared measurements were first made by Harris\textsuperscript{4} and more extensively by Tanner, Sievers and Buhrman.\textsuperscript{5} They found that the far infrared absorption coefficient was several orders of magnitude larger than that predicted by available theories. More recent far infrared measurements have been made by Granqvist, Buhrman, Wyns and Sievers,\textsuperscript{6} and Pramanik, Buhrman, Sievers,\textsuperscript{7} and Russell, Carr and Tanner.\textsuperscript{8}

Theoretically, approaches for inhomogeneous systems have been made from two rather different points of view. Both of these approaches utilize mean field techniques. One of them is a molecular field model originated by Clausius\textsuperscript{9} and Mossotti.\textsuperscript{10} In this approach, one of the components is treated in a fundamentally different manner from the others. This favored component is assumed to serve as a host in which homogeneous inclusions of the other components are dispersed. The first application of this model to optical theories
was made by J.C.M. Garnett. It has also been considered by Barker, Brown, Hashin and Shtrikman, Kerner, Weiner, Cohen, Galeener, Genzel and Martin, Granqvist and Hunderi, and Weaver, Alexander, Teng, Mann, and Bell. The other approach, originated by Bruggeman treats each component on an equal basis in a self-consistent fashion. Generalizations of this approach to optical frequencies have been made by Stroud and Pan, Wood and Ashcroft, and Landauer.

Recently, several proposals have been made to explain the anomalously high far-infrared absorption. Quantized energy levels have been considered by Granqvist, Buhrman, Wyns and Sievers, and Wood and Ashcroft. The absorption by oxide coatings on the metal particles has been discussed by Simanek and Ruppin. Eddy currents have been considered by both Russell, Carr, and Tanner and Granqvist. Correlations of the particle locations can also affect properties of the composite material. These effects have been considered by both Simanek and Ruppin.

This dissertation will discuss some theoretical and experimental work in the area of the optical properties of small-particle systems. The theoretical work will focus on both an extension of static field
theories to finite frequencies and on correlations in the locations of conducting particles. The correlations that are considered here are those that result in conducting clusters of particles. This theoretical work differs from that of earlier workers in that: 1) the electric and magnetic polarizabilities are obtained from the Mie theory fields; 2) the aggregation of the particles into clusters is accounted for when the effective magnetic permeability of the mixture is calculated; and 3) the volume weighted cluster diameter distribution is used when the polarizabilities of the metal are obtained. The experimental work attempts to separate the effects of the bulk electrical properties of the component materials from purely geometric factors.

The organization of this dissertation is as follows. Chapter II contains the details of the theoretical work while Chapter III describes the experimental techniques. Chapter IV describes corrections for several systematic complications and a comparison of theory and experiment, and Chapter V gives the conclusions. There are two appendices. Appendix A reviews the properties of sinusoidally varying fields. Appendix B consists of a listing of major computer programs written for this study.
CHAPTER II

THEORY

Introduction

The proper approach for obtaining the effective dielectric function and magnetic permeability of a system of two or more components has been the subject of much discussion. Of the many methods that have been suggested, the Maxwell Garnett Theory, MGT, and Bruggeman's symmetrical effective medium theory, EMA, are the only methods considered in this dissertation. The discussion here is focused on the MGT.

These two theories share some similarities. They both use an effective medium. An effective medium is a homogeneous medium with the same electromagnetic properties as the inhomogeneous multi-component system. The relative electric and magnetic polarizabilities of an object embedded in a medium with electromagnetic properties different from its own is central to both theories. These relative polarizabilities are the
difference between the absolute polarizabilities of the object and the absolute polarizabilities the same volume would exhibit if it were filled with the host material.

This chapter is organized as follows:

1) The relative electric and magnetic polarizabilities of a sphere is derived using the Mie solution for the internal and external fields.

2) Both the electric and magnetic versions of the MGT are derived.

3) A simple derivation of the electric case of the EMA is given.

4) The low filling fraction limit of the MGT (which is known to be identical to the low filling fraction limit of the EMA) is given.

5) Several different models for the effective electromagnetic constants of a mixture of metal and insulator powders are discussed. The absorption coefficients predicted by each of these models have been calculated numerically.

A. **Polarization of a Sphere**

In uniform fields, the relative polarizability of an object is the relative dipole moment per volume
divided by the incident field. To account for small variations in the incident field over the dimensions of the body, the relative polarizability of a body at finite wavelengths is defined to be the ratio of the average relative dipole moment to the integral of the incident field. The average is taken over the entire body. The discussion here is still further restricted to bodies with dimensions much smaller than the wavelength of the incident radiation.

In general, the relative polarizabilities are tensors. For the case of a spherical body, however, the relative dipole moments are parallel to the incident fields for both the electric and magnetic cases. The relative polarizabilities of a sphere are, therefore, expressed as scaler quantities.

The relative electric, $\gamma$, and magnetic, $\beta$, polarizabilities of a sphere have been calculated from Mie's solution for the internal and external fields of a sphere in an electromagnetic field. For low frequency fields, these expressions yield the same numerical values as those obtained from simpler theories.
1. Simple Expressions

Jackson\textsuperscript{29} and others\textsuperscript{30,31} have found the relative electric polarizability of a dielectric sphere in a static electric field to be

\[ \gamma = \frac{3}{4\pi} \left( \frac{\varepsilon - \varepsilon_h}{\varepsilon + \varepsilon_h} \right) \]  

(1)

where \( \varepsilon_h \) and \( \varepsilon \) are the dielectric constants of the material surrounding the sphere and the sphere, respectively. This expression, when used for nonzero but low frequencies, is known as the quasi-static approximation, qsa.

Jackson\textsuperscript{32} also gives the relative magnetic polarizability of a magnetic, nonconducting sphere with a radius much smaller than the wavelength of the applied magnetic field.

\[ \beta = \frac{3}{4\pi} \left( \frac{\mu - \mu_h}{\mu + 2\mu_h} \right) \]  

(2)

where \( \mu \) and \( \mu_h \) are the magnetic permeabilities of the sphere and the host respectively. Eddy currents are a more important source of magnetization in the case of a conducting sphere. Landau and Lifshitz\textsuperscript{33} have
given an expression for the magnetic polarizability of a conducting sphere of radius $a$ and index of refraction $N = \sqrt{\epsilon}$ in a magnetic field with a frequency $\omega$ and a wavelength much longer than the radius of the sphere.

$$\beta = \frac{-3}{8\pi} \left[ 1 - \frac{3c^2}{(N\omega a)^2} + \frac{3c}{N\omega a} \cot(N\omega a/c) \right]$$  \hspace{1cm} (3)

The expression has two limitations: 1) It assumes that the sphere is immersed in a vacuum. The generalization to the case where the sphere is immersed in an arbitrary medium is not immediately obvious; 2) The derivation neglects the electric field associated with the magnetic field. This electric field affects the magnetic polarizability by modifying the current distribution inside the sphere. These changes to the magnetic polarizability are important at high frequencies even if the wavelength of the external field is still large compared to the sphere radius.

2. **Polarizabilities From Mie Theory**

   a) Mie's solution for a sphere in an electromagnetic field.

   The internal and external fields present when a conducting sphere is placed in an electromagnetic field
were first obtained by Mie in 1908. In the following discussion, the notation and phase conventions correspond roughly to those used by Van de Hulst. The solution here, unlike that of Van de Hulst, does not assume that the sphere is embedded in a vacuum. In addition, an $e^{-i\omega t}$ rather than an $e^{+i\omega t}$ time dependence has been used. A similar solution has been given by Born and Wolf. The solution for the fields in the presence of a perfectly conducting sphere is discussed by Sengupta.

This problem can be simplified by carefully choosing the coordinate axes. The origin of the coordinate system is located at the center of the sphere. The $\hat{x}$ axis is oriented along the direction of the incident electric field. The $-\hat{y}$ axis is oriented along the direction of the incident magnetic field. The incident wave propagates in the $-\hat{z}$ direction. The symmetry of the problem makes it convenient to also introduce spherical coordinates as shown in Figure 1. It is also convenient to set the amplitude of the applied field equal to the index of refraction of the material surrounding the sphere. This somewhat strange normalization simplifies the form of the internal and scattered external fields.

$$\hat{E}_{\text{inc}} = \hat{x} N e^{-i(N_c^\omega)z} e^{-i\omega t}$$ (4)
Figure 1. Coordinate axes used in Mie's solution for a sphere in an electromagnetic field.
The electric and magnetic fields are solutions to
the vector wave equation.

\[ \nabla^2 \vec{E} + (\omega^2 \frac{N^2}{c^2}) \vec{E} = 0 \]  (6)

\[ \nabla^2 \vec{H} + (\omega^2 \frac{N^2}{c^2}) \vec{H} = 0 \]  (7)

The solutions of these equations can be conveniently
expressed in terms of two linearly independent solu­
tions to a scalar wave equation:

\[ \nabla^2 \phi + (\omega^2 \frac{N^2}{c^2}) \phi = 0 \]  (8)

where \( \phi \) is either of these scalar solutions. One of
these solutions, \( u \), corresponds to the case TE, where
the electric field is transverse. The other solution,
\( v \), corresponds to the case TM, where the magnetic
field is transverse. In terms of there scalar
potentials, the electric and magnetic fields are
given by

\[ \hat{E} = \hat{M}_v + i \hat{n}_u \]  (9)

and \[ \hat{B} = \hat{N} (\hat{M}_u - i \hat{n}_v) \]  (10)

The vector quantities \( \hat{M} \) and \( \hat{n} \) are related to the
potentials \( u \) and \( v \) by
\[ \vec{M}_\phi = \text{curl} (\vec{\phi}) \]  

(11)

and

\[ \vec{n}_\phi = \frac{c}{NW} \text{curl} \vec{M}_\phi \]  

(12)

where \( \phi \) is the appropriate potential \( u \) or \( v \). These scalar potentials can be expressed by the following infinite series:

**Incident Fields:**

**TM:** \( u_{\text{inc}} = N_n e^{-i\omega t} \cos \phi \sum_{n=1}^{\infty} (-i)^n \frac{(2n+1)}{n(n+1)} \frac{1}{p_n} (\cos \theta) \times \) \( j_n (N_n \omega r/c) \)  

(13)

**TE:** \( v_{\text{inc}} = N_n e^{-i\omega t} \sin \phi \sum_{n=1}^{\infty} (-i)^n \frac{(2n+1)}{n(n+1)} \frac{1}{p_n} (\cos \theta) \times \) \( j_n (N_n \omega r/c) \)  

(14)

**Scattered Fields:**

**TM:** \( u_s = N_n e^{-i\omega t} \cos \phi \sum_{n=1}^{\infty} (-a_n)(-i)^n \frac{(2n+1)}{n(n+1)} \frac{1}{p_n} (\cos \theta) \times \) \( h_n (N_n \omega r/c) \)  

(15)

**TE:** \( v_s = N_n e^{-i\omega t} \sin \phi \sum_{n=1}^{\infty} (-b_n)(-i)^n \frac{(2n+1)}{n(n+1)} \frac{1}{p_n} (\cos \theta) \times \) \( h_n (N_n \omega r/c) \)  

(16)

**Internal Fields:**

**TM:** \( u_i = N e^{-i\omega t} \cos \phi \sum_{n=1}^{\infty} c_n (-i)^n \frac{(2n+1)}{n(n+1)} \frac{1}{p_n} (\cos \theta) \times \) \( j_n (N_n \omega r/c) \)  

(17)
$v_i = N e^{-i\omega t}\sin\phi \sum_{n=1}^{\infty} d_n(-i)^n \frac{(2n+1)}{n(n+1)} P_n^1(\cos\theta) \times (18)$

$x \ n_j(N\omega r/c)$

In these expressions, $N_h$ and $N$ are the indices of refraction in the material outside and inside the sphere respectively, $j_n$ and $h_n^{(1)}$ are the spherical Bessel functions and spherical Hankel functions of the first kind respectively, and $P_n^1(x)$ are associated Legendre functions. There are several different phase conventions for the associated Legendre functions. The phase convention used here is such that

$$P_n^1(x) = \frac{(1-x^2)^{1/2}}{2^n n!} \frac{d^{n+1}}{dx^{n+1}} (x^2 - 1)^n \quad (19)$$

The expansion coefficients, $a_n$, $b_n$, $c_n$ and $d_n$, are generally known as Mie coefficients. They are determined by the boundary conditions at the surface of the sphere. Sufficient conditions for the continuity of the tangential components of $E$ at the sphere's surface are

$$\frac{1}{N_h} \left( \frac{\partial}{\partial r} \left[ u_{\text{inc}} + u_s \right] \right)_{r=a} = \frac{1}{N} \left( \frac{\partial}{\partial r} u_i \right)_{r=a} \quad (20)$$
and \((v_{\text{inc}} + v_s)_{r=a} = (v_1)_{r=a}\) \(\quad (21)\)

Sufficient conditions for the continuity of the tangential components of \(\vec{H}\) are

\[N_h (u_{\text{inc}} + u_s)_{r=a} = N u_i_{r=a}\] \(\quad (22)\)

\[
\left(\frac{\partial (r[v_{\text{inc}} + v_s])}{\partial r}\right)_{r=a} = \left(\frac{\partial (rv_i)}{\partial r}\right)_{r=a}
\] \(\quad (23)\)

The Mie coefficients are customarily expressed in terms of the Riccati-Bessel functions \(\psi\) and \(\zeta\),

\[\psi_n(x) = x j_n(x)\] \(\quad (24)\)

\[\zeta_n(x) = x h_n^{(1)}(x)\] \(\quad (25)\)

For TM modes:

Outside: \(\quad a_n = \frac{\left(\frac{N_n}{N_h}\right) \psi_n(N_h \omega a/c) \psi_n(N \omega a/c) - \psi_n(N \omega a/c) \psi_n(N_h \omega a/c)}{\left(\frac{N_n}{N_h}\right) \psi_n(N \omega a/c) \zeta_n(N_h \omega a/c) - \psi_n(N \omega a/c) \zeta_n(N_h \omega a/c)}\)

For TE modes:

Outside: \(\quad b_n = \frac{\left(\frac{N_n}{N_h}\right) \psi_n(N \omega a/c) \psi_n(N_h \omega a/c) - \psi_n(N_h \omega a/c) \psi_n(N \omega a/c)}{\left(\frac{N_n}{N_h}\right) \psi_n(N \omega a/c) \zeta_n(N_h \omega a/c) - \psi_n(N \omega a/c) \zeta_n(N_h \omega a/c)}\)

For TM modes:

Inside: \(\quad c_n = \left(\frac{N_n}{N_h}\right) \left(\frac{\psi_n(N_h \omega a/c) - a_n \zeta_n(N_h \omega a/c)}{\psi_n(N \omega a/c)}\right)\) \(\quad (28)\)

Inside: \(\quad c_n = \left(\frac{N_n}{N_h}\right) \left(\frac{\psi_n(N_h \omega a/c) - a_n \zeta_n(N_h \omega a/c)}{\psi_n(N \omega a/c)}\right)\) \(\quad (28)\)
where $\mu_h$ and $\mu$ are the magnetic permeabilities of the material outside and inside the sphere respectively and the primes denote differentiation with respect to the argument. The magnetic permeabilities have been included in these expressions for reference only. For all of the bulk materials considered in this investigation, the magnetic permeabilities were equal to unity. The first few values for the Mie coefficients for scattering from a sphere immersed in a vacuum are given in Table 1 for selected values of the internal dielectric constant.

The cartesian expressions for the incident electric and magnetic fields, equations 4 and 5 will be needed to find the polarizabilities. The series expression for the internal and external electric fields in spherical coordinates will also be needed. The latter fields are given below. The series expressions for the magnetic fields in spherical coordinates will not be needed.
TABLE 1

Mie Coefficients for 70 cm\(^{-1}\) radiation incident on a palladium sphere immersed in vacuum.
Conductivity A: room temperature, bulk value
Conductivity B: 10 times room temperature, bulk value

<table>
<thead>
<tr>
<th>Sphere Diameter</th>
<th>Conductivity</th>
<th>Order (n)</th>
<th>Mie Coefficients</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>a(_n)</td>
<td>b(_n)</td>
</tr>
<tr>
<td>1(\mu)M</td>
<td>A 1</td>
<td>(5.8\times10^{-10})</td>
<td>(17.1\times10^{-6})</td>
</tr>
<tr>
<td>2</td>
<td>(7.6\times10^{-15})</td>
<td>(-11.7\times10^{-11})</td>
<td>(3.2\times10^{-11})</td>
</tr>
<tr>
<td>3</td>
<td>(7.2\times10^{-20})</td>
<td>(-12.1\times10^{-15})</td>
<td>(4.3\times10^{-16})</td>
</tr>
<tr>
<td>4</td>
<td>--</td>
<td>--</td>
<td>(-1.9\times10^{-15})</td>
</tr>
<tr>
<td>10(\mu)M</td>
<td>A 1</td>
<td>(5.7\times10^{-5})</td>
<td>(-17.2\times10^{-3})</td>
</tr>
<tr>
<td>2</td>
<td>(5.9\times10^{-12})</td>
<td>(-12.1\times10^{-8})</td>
<td>(1.0\times10^{-9})</td>
</tr>
<tr>
<td>3</td>
<td>(3.3\times10^{-15})</td>
<td>(-11.5\times10^{-11})</td>
<td>(9.8\times10^{-13})</td>
</tr>
<tr>
<td>4</td>
<td>--</td>
<td>--</td>
<td>(-1.9\times10^{-15})</td>
</tr>
<tr>
<td>1(\mu)M</td>
<td>B 1</td>
<td>(1.4\times10^{-10})</td>
<td>(-17.1\times10^{-6})</td>
</tr>
<tr>
<td>2</td>
<td>(1.3\times10^{-15})</td>
<td>(-12.7\times10^{-11})</td>
<td>(7.4\times10^{-12})</td>
</tr>
<tr>
<td>3</td>
<td>(1.1\times10^{-20})</td>
<td>(-12.1\times10^{-15})</td>
<td>(1.2\times10^{-16})</td>
</tr>
<tr>
<td>4</td>
<td>--</td>
<td>--</td>
<td>(5.8\times10^{-20})</td>
</tr>
<tr>
<td>10(\mu)M</td>
<td>B 1</td>
<td>(5.3\times10^{-5})</td>
<td>(-17.2\times10^{-3})</td>
</tr>
<tr>
<td>2</td>
<td>(1.5\times10^{-9})</td>
<td>(-11.7\times10^{-5})</td>
<td>(9.5\times10^{-8})</td>
</tr>
<tr>
<td>3</td>
<td>(1.0\times10^{-12})</td>
<td>(-12.1\times10^{-8})</td>
<td>(1.8\times10^{-10})</td>
</tr>
<tr>
<td>4</td>
<td>(5.7\times10^{-16})</td>
<td>(-11.5\times10^{-11})</td>
<td>(1.8\times10^{-13})</td>
</tr>
</tbody>
</table>
Table 2. Special functions used in Mie Theory

<table>
<thead>
<tr>
<th>Order $n$</th>
<th>$P_n^1(\cos \theta)$</th>
<th>$j_n(z)$</th>
<th>$h_n^{(1)}(z)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>$\sin \frac{z}{z}$</td>
<td>$(\sin z - i \cos z)/z$</td>
</tr>
<tr>
<td>1</td>
<td>$\sin \theta$</td>
<td>$\sin \frac{z}{z^2} - \cos \frac{z}{z}$</td>
<td>$(\sin \theta - i \cos \frac{z}{z})/z^2$ + $(-\cos z + i \sin \frac{z}{z})/z$</td>
</tr>
<tr>
<td>2</td>
<td>$3 \sin \theta \cos \theta$</td>
<td>$(3/z^3 - 1/z)\sin z - 3 \cos \frac{z}{z^2}$</td>
<td>$(\sin z - i \cos \frac{z}{z})(3/z^2 - 1/z) - 3(\cos z + i \sin \frac{z}{z})/z^2$</td>
</tr>
</tbody>
</table>
Table 3. Small argument approximations
for $j_n(z)$ and $h_n^{(1)}(z)$

<table>
<thead>
<tr>
<th>Order</th>
<th>$j_n(z)$</th>
<th>$h_n^{(1)}(z)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>$1 - i/z$</td>
</tr>
<tr>
<td>1</td>
<td>$z/3$</td>
<td>$z/3 - i/z^2$</td>
</tr>
<tr>
<td>2</td>
<td>$z^2/15$</td>
<td>$z^2/15 - i3/z^3$</td>
</tr>
</tbody>
</table>
Incident Field:

\[ E_r = N_h e^{-i\omega t \cos \phi} \sum_{n=1}^{\infty} (-i)^n \frac{(2n+1)}{n(n+1)} P_n^1(\cos \theta) \times \]

\[ \times \left[ \psi_n(N_h\omega r/c) + \psi_n(N_h\omega r/c) \right] \]  \hspace{0.5cm} (30)

\[ E_\theta = N_h e^{-i\omega t \cos \phi} \sum_{n=1}^{\infty} (-i)^n \frac{(2n+1)}{n(n+1)} \left[ \frac{P_n^1(\cos \theta) \psi_n(N_h\omega r/c)}{\sin \phi} \right] \]

\[ + i \frac{\partial P_n^1(\cos \theta)}{\partial \theta} \frac{\psi_n(N_h\omega r/c)}{(N_h\omega r/c)} \]  \hspace{0.5cm} (31)

\[ E_\phi = -N_h e^{-i\omega t \sin \phi} \sum_{n=1}^{\infty} (-i)^n \frac{(2n+1)}{n(n+1)} \left[ \frac{\partial P_n^1(\cos \theta)}{\partial \theta} \frac{\psi_n(N_h\omega r/c)}{\sin \phi} \right] \]

\[ + i \frac{P_n^1(\cos \theta)}{\sin \phi} \frac{\psi_n'(N_h\omega r/c)}{(N_h\omega r/c)} \]  \hspace{0.5cm} (32)
Scattered Field:

\[ E_r = N_h e^{-i \omega t} \cos \phi \sum_{n=1}^{\infty} (-i)^n \frac{(2n+1)}{n(n+1)} (-a_n) P_n^1(\cos \theta) \times \]

\[ \times \left[ \zeta_n'' (N_h r/c) + \zeta_n (N_h \omega r/c) \right] \quad (33) \]

\[ E_\theta = -N_h e^{-i \omega t} \cos \phi \sum_{n=1}^{\infty} (-i)^n \frac{(2n+1)}{n(n+1)} \times \]

\[ \times \left[ i a_n \frac{\partial P_n^1(\cos \theta)}{\partial \theta} \frac{\zeta_n'(N_h r/c)}{(N_h \omega r/c)} + b_n P_n^1(\cos \theta) \frac{\zeta_n(N_h \omega r/c)}{(N_h \omega r/c)} \right] \quad (34) \]

\[ E_\phi = N_h e^{-i \omega t} \sin \phi \sum_{n=1}^{\infty} (-i)^n \frac{2n+1}{n(n+1)} \left[ ia_n \frac{P_n^1(\cos \theta)}{\sin \theta} \frac{\zeta_n'(N_h \omega r/c)}{(N_h \omega r/c)} + b_n \frac{P_n^1(\cos \theta)}{\partial \theta} \frac{\zeta_n(N_h \omega r/c)}{(N_h \omega r/c)} \right] \quad (35) \]
Internal Fields:

\[ E_r = N \exp(-i\omega t) \cos \phi \sum_{n=1}^{\infty} (-i)^n \frac{n(2n+1)}{n(n+1)} c_n \frac{P_n^1(\cos \theta)}{n} \times \]
\[ \times \left[ \psi_n''(N\omega r/c) + \psi_n'(N\omega r/c) \right] \]  \hspace{1cm} (36)

\[ E_\theta = N \exp(-i\omega t) \cos \phi \sum_{n=1}^{\infty} (-i)^n \frac{n(2n+1)}{n(n+1)} \left[ ic_n \frac{\partial P_n^1(\cos \theta)}{\partial \theta} \frac{\psi_n'(N\omega r/c)}{(N\omega r/c)} \right. \]
\[ + d_n \frac{P_n^1(\cos \theta)}{\sin \theta} \frac{\psi_n'(N\omega r/c)}{(N\omega r/c)} \left. \right] \]  \hspace{1cm} (37)

\[ E_\phi = -N \exp(-i\omega t) \sin \phi \sum_{n=1}^{\infty} (-i)^n \frac{n(2n+1)}{n(n+1)} \times \]
\[ \times \left[ ic_n \frac{P_n^1(\cos \theta)}{\sin \theta} \frac{\psi_n'(N\omega r/c)}{(N\omega r/c)} \right. \]
\[ + d_n \frac{\partial P_n^1(\cos \theta)}{\partial \theta} \frac{\psi_n'(N\omega r/c)}{(N\omega r/c)} \left. \right] \]  \hspace{1cm} (38)
b) Electric Polarizability from the Mie fields.

The relative electric polarizability can be calculated from the internal and external electric fields given in the last section. The relative electric dipole moment, \( \vec{d} \), is given by

\[
\vec{d} = \oint_v \vec{x} \rho_{\text{pole}} \, dv = \frac{1}{4\pi} \oint_v \vec{x}(\nabla \cdot \vec{E}) \, dv
\]  

(39)

where \( V \) is the volume of the sphere and \( \rho_{\text{pole}} \) is the polarization charge density.

The electric field, \( \vec{E} \), can be written as

\[
\vec{E} = \vec{E}_{\text{internal}} + S(r-a) \vec{E}_{\text{external}} - \vec{E}_{\text{internal}}
\]  

(40)

where \( S(x) \) is the unit step function.

\[
S(x) = \begin{cases} 
0 & x < 0 \\
1 & x \geq 0 
\end{cases}
\]  

(41)

Therefore,

\[
\vec{d} = \frac{1}{4\pi} \oint_v \vec{x} \left[ \vec{E}_{\text{external}} - \vec{E}_{\text{internal}} \right] \delta(r-a) \, dv.
\]  

(42)

This expression does in fact represent the relative electric dipole moment because the differences in the polarization between the media cause the polarization charge to collect on the boundary. This polarization charge gives a discontinuity in the normal component of the electric fields. By using the electric
fields in the last section, it can be shown that

\[ \hat{\mathbf{d}} = \hat{x} \frac{ca^2}{\omega} e^{-i\omega t} \left[ j_1(N_h\omega/c) \\
- a_1h_1^{(1)}(N_h\omega/c) - C_1j_1(N\omega/c) \right] \quad (43) \]

Due to the symmetry of the problem, only the first TM term out of all the terms in the infinite series (eqs 13-18) contributes to the average relative electric dipole moments. The integral of the incident electric field is

\[ \int_{E_{inc}}^{\hat{E}} \mathbf{d}V = \hat{x} \frac{4\pi ca^2}{\omega} e^{-i\omega t} j_1(N_h\omega/c) \quad (44) \]

Notice that the average relative dipole moment is parallel to the integral of the incident electric field. The relative electric polarizability is

\[ \gamma = \frac{1}{4\pi j_1(N_h\omega/c)} \left[ j_1(N_h\omega/c) - a_1h_1^{(1)}(N_h\omega/c) \\
- C_1j_1(N\omega/c) \right] \quad (45) \]

c) **Magnetic Polarizability from the Mie Fields**

The magnetic dipole moment, \( \hat{\mathbf{m}} \), can be calculated from the current inside the sphere. This current is related to the internal electric field by Ohm's law.

\[ \hat{\mathbf{m}} = \frac{1}{2c} \int_{V} [\hat{x} \times \hat{\mathbf{j}}] \mathbf{d}V \quad (46) \]

\[ = \frac{i\omega (N^2 - \mu)}{8\pi c\mu} \int_{V} [\hat{x} \times \hat{\mathbf{E}}] \mathbf{d}V \quad (47) \]
where V is the volume of the sphere and \( \mu \) is the magnetic permeability of the sphere. This expression is not the correct one for the relative magnetic dipole moment if the host is conducting and only represents that portion of the magnetic moment that results from eddy currents. It does represent the relative magnetic dipole moment of the type of materials considered in this study; specifically it represents nonmagnetic spheres embedded in a nonmagnetic, insulating host. Since the dipole moment is generated by eddy currents, it can be nonzero even if the sphere is nonmagnetic. Evaluating the integral in the above expression with the fields given in the last section,

\[
\mathbf{m} = -\gamma (N^2 - \mu) \frac{d_1 a^3 e^{-i\omega t}}{2\mu} \left[ \frac{3 j_1(N\omega a/c) - j_0(N\omega a/c)}{(N\omega a/c)} \right]
\]

(48)

In a manner similar to that in the electric case, the symmetry of the problem results in only one term of the infinite series contributing to the volume average. In this case it is the first TE term. The integral of the incident magnetic field is

\[
\int_{V} H_{\text{inc}} \, dv = -\gamma N_{h} \frac{4\pi c a^2 e^{-i\omega t} j_1(N_{h}\omega a/c)}{\mu_{h} \omega}
\]

(49)
As in the electric case, the average dipole moment is parallel to the integral of the incident field. The magnetic polarizability is

\[
\beta = \frac{d_1 N_0 \omega a (N - \mu)}{8 \pi c N \omega j_1 (N_0 \omega a/c)} \left[ \frac{3 j_1 (N_0 \omega a/c) - j_0 (N_0 \omega a/c)}{(N_0 \omega a/c)} \right]
\]

(50)

3. Comparison of the Mie Polarizabilities with the Simple Expressions

It is of the interest to compare the polarizabilities obtained from the Mie fields with the quasi-state electric (eq. 1) and the Landau and Lifshitz magnetic (eq. 3) polarizabilities mentioned at the beginning of the chapter. These comparisons will be made by performing some numerical calculations. A Drude model, dielectric function

\[
\varepsilon = 1 - \frac{\omega_p^2}{\omega^2 + \frac{i\omega}{\tau}}
\]

(51)

will be used for spheres. In this expression, \(\omega_p\) is the plasma frequency, which will be taken to be that of Pd (\(\hbar\omega_p = 5.97 \text{eV}\)) because Pd was the metallic component of the majority of the experimental samples, while \(\tau\) will be varied to adjust the conductivity of the sphere. For simplicity, these calculations will assume that the sphere is surrounded by vacuum.

Curves are shown for relaxation times chosen such that the conductivity was one or 10 times that of
Pd at room temperature. The curves marked A represent the Mie Theory values while the curves marked B represent the simple theory values.

a) **Electric Case**

Figures 2 and 3 show the size and frequency dependence of the real part of the electric polarizability. This quantity is positive definite and reduces to $\frac{3}{4\pi}$, the static electric polarizability of a perfectly conducting sphere at low frequencies and diameters. The quasi-static value is independent of both frequency and particle diameter. The Mie theory value is also essentially frequency independent. It does rise slightly, though, for large particle diameters. However, for the frequency and diameter regions of interest here, the deviation between the Mie theory and quasi-static values never exceeds a few percent of the quasi-static value. The real part of the polarizability shows no dependence on the bulk conductivity of the metal.

Figures 4, 5 and 6 show the size and frequency dependence of the imaginary part of the electric polarizability. For low frequencies, this quantity
Figure 2. The real part of the electric polarizability versus sphere diameter at 70 cm$^{-1}$ for palladium spheres

Curve A: Mie theory  
B: Quasi-static theory

The same curves are obtained when either the room temperature, bulk conductivity or 10 time the room temperature bulk conductivity is used.
Figure 3. The real part of the electric polarizability versus wavenumber for 1 μm diameter palladium spheres. Both the quasi-static and the Mie theories yield the same results when either the room temperature, bulk conductivity or 10 times the room temperature, bulk conductivity is used.
Figure 4. The imaginary part of the electric polarizability versus sphere diameter at 70 cm$^{-1}$ for palladium spheres.

Curve A: Mie theory
B: Quasi-static theory

Solid lines: Room temperature, bulk conductivity

Dotted lines: 10 times the room temperature, bulk conductivity
Figure 4. The imaginary part of the electric polarizability versus sphere diameter at 70 cm$^{-1}$ for palladium spheres.

Curve A: Mie theory
B: Quasi-static theory

Solid lines: Room temperature, bulk conductivity

Dotted lines: 10 times the room temperature, bulk conductivity
Figure 5. Enlarged view of the imaginary part of the electric polarizability versus sphere diameter at 70 cm\(^{-1}\) for palladium spheres

Curve A: Mie theory  
B: Quasi-static theory

Solid lines: room temperature, bulk conductivity

Dotted lines: 10 times the room temperature, bulk conductivity
Figure 6. The imaginary part of the electric polarizability versus wavenumber for 1 μm diameter palladium spheres

Curve A: Mie theory  
B: Quasi-static theory

Solid lines: room temperature, bulk conductivity  
Dotted lines: 10 times the room temperature, bulk conductivity
vanishes. It increases with increasing frequency or particle size. The Mie theory value is considerably larger than the corresponding quasi-static value. This deviation is over two values of magnitude for 10 μm particles at 70 cm\(^{-1}\). Both theories predict that the imaginary part of the electric polarizability will decrease with increased sphere conductivity. When the conductivity is raised from its room temperature bulk value by a factor of 10. The Mie theory value of a 1 μm sphere at 70 cm\(^{-1}\) decreases by a factor of about 3.5 while the quasi-static value decreases by exactly 10.

b) Magnetic Case

The real part of the magnetic polarizability \(\beta_1\) is negative and vanishes for low frequencies and small particle diameters as is shown in Figures 7 and 8. Eddy currents therefore cause the sphere to be diamagnetic as one would expect. This part of the polarizability decreases as the conductivity is increased by an order of magnitude from its room temperature, bulk value. The real part of the Mie polarizability is somewhat smaller in magnitude than the corresponding Landau and Lifshitz value for large particles.
Figure 7. The real part of the magnetic polarizability versus sphere diameter at 70 cm$^{-1}$ for palladium spheres.

Curve A: Mie theory  
B: Landau and Lifshitz theory

Solid lines: room temperature, bulk conductivity

Dotted lines: 10 times the room temperature, bulk conductivity
Figure 8. The real part of the magnetic polarizability versus wavenumber for 1 µm palladium spheres. Both the Mie and the Landau and Lifshitz theories yield the same results for this quantity.

Solid line: room temperature, bulk conductivity

Dotted line: 10 times the room temperature, bulk conductivity
The imaginary part of the magnetic polarizability, $\beta_2$ is positive definite and at least twice as large as the imaginary part of the electric polarizability over the entire frequency and diameter regions of interest. This quantity is shown in Figures 9 and 10. The optical absorption is therefore dominated by the magnetic contribution. For low frequencies and small diameters, the Mie and the Landau and Lifshitz theories yield the same results. The Mie theory result is larger than the Landau and Lifshitz result when the frequency or the diameter is large. This deviation increases as the conductivity of the metal increases. For high frequencies, large diameters, and high conductivities, the deviation between the two theories can exceed an order of magnitude.

There is a peak in both the frequency and size dependence of the imaginary part of the magnetic polarizability which is related to the classical skin depth. As the conductivity of the sphere is increased, the peaks shifts to lower frequencies and smaller diameters. However, the magnitude of this peak decreases with increased conductivity. The small diameter region of the polarization versus diameter curve is shown with an expanded scale in Figure 11. The movement of the peak toward larger diameters
Figure 9. The imaginary part of the magnetic polarizability versus sphere diameter at 70 cm$^{-1}$ for palladium spheres.

Curve A: Mie theory
B: Landau and Lifshitz theory

Solid lines: room temperature, bulk conductivity

Dotted lines: 10 times the room temperature, bulk conductivity
Figure 10. Enlarged view of the imaginary part of the magnetic polarizability versus sphere diameter at 70 cm\(^{-1}\) for palladium spheres. Both the Mie and the Landau and Lifshitz theories yield the same results for small spheres.

Solid line: room temperature, bulk conductivity

Dotted line: 10 times the room temperature, bulk conductivity
Figure 11. The imaginary part of the magnetic polarizability for 1 μm diameter palladium spheres. Both the Mie and the Landau and Lifshitz theories yield the same results for small spheres.

Solid line: room temperature, bulk conductivity

Dotted line: 10 times the room temperature, bulk conductivity
causes the polarization of very small particles to decrease while that of very large particles increases. This shift will be of interest when the optical absorption of the hydrogenated samples is discussed.

B. Effective Medium Theories

The purpose of an effective medium theory is to determine the electromagnetic properties of a composite material. The differences between the two theories presented here arise from different assumptions about the nature of the composite material. As a result of different assumptions, the EMA treats each component on an equal footing while the MGT distinguishes between the components.

1. Maxwell Garnet Approximation

In the MGT, inclusions of a single component are assumed to be embedded in a host component. From the very outset, the host component is definitely distinguished from the other components. The MGT expressions for the dielectric function and the magnetic permeability are similar in form. The electric case will be considered first and then the magnetic case will be obtained by analogy.
a) **Electric Case**

The effective dielectric function of a composite can be obtained by studying the internal fields. The electric field inside a sample of a dielectric material depends on both the field outside the sample and the sample geometry. The analysis of the internal fields can be simplified by a careful choice of both the sample geometry and the field applied to the outside of the sample. The situation considered here will consist of a rectangular slab of the composite placed between the plates of a parallel plate capacitor. Two of the sample faces are parallel to the capacitor plate. The sample is assumed to be sufficiently large that edge effects can be neglected. In the region of interest, both the external and internal fields are perpendicular to the capacitor plates. For comparison purposes, a sample of the host material is subject to the same applied field inside an identical capacitor.

The polarizations inside each material are

\[
\vec{P}_n = \left(\frac{1}{4\pi}\right)(\vec{P}_n^0 - \vec{E}_n)
\]  
(52)

and

\[
\vec{P}_{\text{eff}} = \left(\frac{1}{4\pi}\right)(\vec{P}_{\text{eff}}^0 - \vec{E}_{\text{eff}})
\]  
(53)
where \( \vec{P}_h, \vec{D}_h, \) and \( \vec{E}_h \) are the polarization, displacement, and electric fields respectively inside the host. \( \vec{P}_{\text{eff}}, \vec{D}_{\text{eff}}, \) and \( \vec{E}_{\text{eff}} \) are the average polarization, average displacement, and average electric fields inside the composite. From the boundary conditions on the normal component of the displacement vector at the surface of the sample,

\[
\vec{D}_h = \vec{D}_{\text{eff}} = \vec{E}_0 \quad (54)
\]

where \( \vec{E}_0 \) is the electric field between the capacitor plate in the absence of the sample materials.

\[
\Delta \vec{P} = \vec{P}_{\text{eff}} - \vec{P} = (1/4\pi) (\vec{E}_h - \vec{E}_{\text{eff}}) = (1/4\pi) (\varepsilon_m/\varepsilon_h - 1) \vec{E}_{\text{eff}} \quad (56)
\]

where \( \varepsilon_m \) is the MGT effective dielectric function of the composite and \( \varepsilon_h \) is the dielectric function of the host. The difference in polarization arises because of the polarization of the inclusions.

\[
\Delta \vec{P} = \vec{E}_{\text{loc}} \sum_k f_k \gamma_k \quad (57)
\]

where \( \vec{E}_{\text{loc}} \) is the electric field present at a typical inclusion, \( f_k \) is the volume filling fraction of the \( k^{th} \) component, \( \gamma_k \) is the relative polarizability of the \( k^{th} \) component, and the sum runs over each type of inclusion.
In the following discussion of the local field at a typical inclusion, it may be useful to refer to Figure 12. The local field at a typical inclusion (labeled A on the Figure) is the sum of the applied field, $E_o$, and the fields produced by the polarization changes of the host and the relative polarizations of the other inclusions. Most of the fields produced by the other inclusions cancel each other out. The only inclusion fields acting on A are those produced by the relative polarization charges exposed to A and those exposed to the surface of the sample. The sum of the fields due to the relative polarization charges exposed to the sample surface and the applied field is the average electric field, $E_{\text{eff}}$. To simplify the calculation of the fields due to the relative polarization charges closest to A, a somewhat different model will now be introduced. On this new model, most of the host material and all of the other inclusions are replaced by a uniformly polarized, homogeneous material with the same dielectric function as the effective dielectric function of the composite. (See Figure 13). In this model, A is at the center of a spherical cavity carved into the effective medium. The diameter of this cavity is much less than the wavelength of the
Figure 12. Composite material between the capacitor plates. A typical inclusion is Labeled A.
Figure 13. Composite material after an effective medium was substituted for most of the inclusions and the host material.
radiation inside the effective medium. The space between the inner surface of the cavity and $A$ is filled with the host material. Since the cavity is filled with the host material, the polarization charge on the inner surface of the cavity arise due to the relative polarization, $\Delta F$, of the effective medium. The relative polarization charges of the other inclusions closest to $A$ have been replaced by the polarization charge on the cavity's inner surface. In an average sort of way, this effective medium has the same effect on $A$ as the other inclusions and the host did in the previous model.

The polarization surface charge density, $\sigma$, on the inner surface of the cavity is determined by the relative polarization of the effective medium and the shape of the cavity. It is easy to convince oneself that

$$\sigma \propto \cos \theta.$$ \hspace{1cm} (58)

By adjusting the proportionality constant so that the dipole moment of the cavity is equal to the negative of the product of the relative polarization of the effective medium and the volume of the cavity,

$$\sigma = -(\Delta \mathbf{p}) \cos \theta.$$ \hspace{1cm} (59)
The electric field at a point \((\vec{x}, t)\) due to a charge \(dq\) at another point \((\vec{x}', t')\), where \(t'\) is the retarded time, is given by

\[
\vec{E}(\vec{x}, t) = dq(\vec{x}, t') \frac{(\vec{x} - \vec{x}')}{|\vec{x} - \vec{x}'|^3} \tag{60}
\]

\[
t' = t - \frac{|\vec{x} - \vec{x}'|}{c} \tag{61}
\]

Retardation effects, represented by the second term in equation 61, can be neglected if the cavity is very much smaller than the vacuum wavelength of the radiation. Using the cavity surface charge density, equation 59, and Coulomb's law, equation 60, the electric field at the center of the cavity due to the cavity's surface charge density is

\[
\vec{E}_{\text{cavity}} = \mathcal{E}_0 \int_0^\pi \left( \frac{2\pi}{a^2} \sin^2 \theta \right) \cos \theta \, d\theta \tag{62}
\]

\[
= \frac{4\pi}{3} (\Delta \mathcal{P}) \tag{63}
\]

\[
\vec{E}_{\text{loc}} = \vec{E}_{\text{eff}} + \frac{4\pi}{3} (\Delta \mathcal{P}) \tag{64}
\]

The total field at the center of the cavity can be expressed in terms of the dielectric functions of the host and the effective medium by substituting \((\Delta \mathcal{P})\) from equation 56.

\[
\vec{E}_{\text{loc}} = \mathcal{E}_{\text{eff}} \left( \frac{\varepsilon_m + 2\varepsilon_h}{\varepsilon_h} \right) \tag{65}
\]
The effective dielectric function of the composite, $\varepsilon_m$, can now be expressed in terms of the dielectric function of the host, $\varepsilon_h$, the relative polarizabilities of the inclusions, $\gamma_k$, and the inclusion volume filling fraction, $f_k$.

Combining equations 56, 57 and 65,

$$
\varepsilon_m = \varepsilon_h \left( \frac{1 + (8\pi/3) \sum_k f_k \gamma_k}{1 - \left(\frac{4\pi}{3}\sum_k f_k \gamma_k\right)} \right)
$$

(66)

Up to this point, the derivation has been general in the sense that no static field approximations have been made. The finite frequency MGT dielectric function can be obtained by substituting the Mie theory electric polarizability, equation 46 into the above expression.

The quasi-static approximation is used by many authors.\textsuperscript{3,27} It is obtained by substituting the quasi-static electric polarizability, equation 2, into the MGT dielectric function, equation 66. In this case

$$
\varepsilon_m = \varepsilon_h \left( \frac{1 + 2 \sum_k f_k \left( \frac{\varepsilon_k - \varepsilon_h}{\varepsilon_k + 2\varepsilon_h} \right)}{1 - \sum_k f_k \left( \frac{\varepsilon_k - \varepsilon_h}{\varepsilon_k + 2\varepsilon_h} \right)} \right)
$$

(67)
where $\varepsilon_k$ is the dielectric function of the $k^{th}$ component. The use of this expression at finite frequencies is valid when the quasi-static electric polarizability is a good approximation to the actual polarizability.

ii) **Magnetic Case**

The effective magnetic permeability of a composite can also be obtained by studying the composite's internal fields. The derivation can be shortened considerably by noting several similarities between the electric and magnetic cases. The magnetic field, $\mathbf{H}$, is related to the magnetic induction, $\mathbf{B}$, the magnetic permeability, $\mu$, and the magnetization, $\mathbf{M}$, in the same manner as the electric field, $\mathbf{E}$, is related to the displacement, $\mathbf{D}$, the dielectric function, $\varepsilon$, and the electric polarization, $\mathbf{P}$.

\[
\mathbf{B} = \mathbf{H} + 4\pi \mathbf{M} = \mu \mathbf{H} \tag{68}
\]

\[
\mathbf{D} = \mathbf{E} + 4\pi \mathbf{P} = \varepsilon \mathbf{E} \tag{69}
\]

Both the electric and the magnetic fields are solutions to the same wave equation (equations 6 and 7).
The boundary conditions encountered in the magnetic case are similar to those encountered in the electric case. The quantities \( \hat{n} \cdot \vec{D}, \hat{n} \cdot \vec{E}, \hat{n} \times \vec{F}, \) and \( \hat{n} \times \vec{H} \) are all continuous at a boundary where \( \hat{n} \) is the outward normal. Due to these similarities, the expression for the MGT effective magnetic permeability, \( \mu_m \), can be obtained using the derivation given above for the MGT effective dielectric function if the following substitutions are made:

\[
\begin{align*}
\vec{D} & \rightarrow \vec{E} \\
\vec{E} & \rightarrow \vec{H} \\
\vec{P} & \rightarrow \vec{M} \\
\gamma & \rightarrow B \\
\varepsilon & \rightarrow \beta
\end{align*}
\]

Therefore,

\[
\mu_m = \mu_h \left( \frac{1 + (8\pi/3) \sum_{k} f_k \beta_k}{1 - (4\pi/3) \sum_{k} f_k \beta_k} \right)
\]

where \( \mu_h \) is the magnetic permeability of the host. \( f_k \) is the volume filling fraction and \( \beta_k \) is the magnetic polarizability of the \( k^{th} \) component.
2. Effective Medium Approximation

In Bruggeman's symmetric effective medium approximation, EMA, the components of the composite material are treated in a symmetric fashion. The discussion here will follow that of Landauer. For conceptual purposes, the composite is viewed as a collection of many small, individual, homogeneous grains. In calculating the polarizabilities of a single grain, the grain will be assumed to be embedded in a homogeneous, effective medium which has the same electromagnetic properties as the effective electromagnetic properties of the composite system. The dimensions of each grain are very much smaller than the optical wavelength in the effective medium.

In the presence of external fields, each grain will have net electric and magnetic dipole moments. These moments will cause local deviations in the fields from their average values. The volume averages of these local deviations are:

\[ 4\pi \hat{p} = \overline{E}_{\text{eff}} \sum_k \bar{\gamma}_k \]  

\[ 4\pi \hat{m} = \overline{H}_{\text{eff}} \sum_k \bar{\beta}_k \]  

where \( \hat{p} \) and \( \hat{m} \) are the average electric and magnetic polarizations respectively relative to the effective
medium, \( \gamma_k \) and \( \beta_k \) are the relative electric and magnetic polarizabilities and \( f_k \) is the volume filling fraction of the \( k^{th} \) component. The properties of the effective medium are chosen self-consistently to make these average deviations vanish.

\[
\sum_k f_k \gamma_k = 0 \quad (78)
\]

\[
\sum_k f_k \beta_k = 0 \quad (79)
\]

In principle, the finite frequency electromagnetic properties of a composite can be obtained by substituting the Mie theory polarizabilities into the above expression. In practice, this procedure is more than a little difficult. This dissertation will discuss only the quasi-static electric case which is obtained by substituting the quasi-static electric polarizabilities, equation 2, into the above self-consistency equation. The quasi-static effective dielectric function should yield approximately the correct result for nonzero frequencies if the dimensions of each grain are very much smaller than the skin depth of the bulk material. The quasi-static EMA dielectric function, \( \varepsilon_{QE} \), for a two component system is:
\[ \varepsilon_{QE} = \frac{1}{2} \left( Q \pm (Q^2 + 8 \varepsilon_1 \varepsilon_2) \right)^{1/2} \]  
\text{(80)}

where

\[ Q = (3f_2 - 1)\varepsilon_2 + (3f_1 - 1)\varepsilon_1 \]  
\text{(81)}

In these expressions, the subscripts refer to the components labeled 1 and 2. The sign before the square root is chosen to make the imaginary part of \( \varepsilon_{QE} \) positive.

For the case of a two component metal-insulator mixture, the differences between the MGT and the EMA are readily apparent. Many properties of the mixture such as the dielectric function and the D. C. electrical conductivity exhibit a different dependency on the metal filling fraction, \( f_m \), if the EMA is used instead of the MGT. The D. C. electrical conductivity will serve to illustrate this difference. For \( f_m \) above a critical value of 1/3, the EMA predicts a conducting mixture. It predicts an insulating mixture for \( f_m \) below 1/3. In contrast, if the metal is the host, the MGT predicts a conducting mixture for all nonzero values of \( f_m \). If the insulator is the host, the MGT predicts an insulating mixture for all values of \( f_m \) less than one. This difference arises because the EMA, unlike the MGT, treats the components in a symmetric fashion.
3. **Low Concentration Limit**

The low concentration limit of these effective medium theories is of particular interest in this dissertation because this was the only concentration region that was accessible to experimental measurements. The discussion here will be confined to the MGT. Expanding the denominator of the MGT dielectric function, equation 66, in powers of $\sum f_k \gamma_k$ and keeping only lowest order terms,

$$
\varepsilon_m = \varepsilon_h (1 + 4\pi \sum f_k \gamma_k)
$$

Similarly,

$$
\mu_m = \mu_h (1 + 4\pi \sum f_k \beta_k)
$$

Of particular interest is the low concentration expression for the absorption coefficient for waves propagating in the inhomogeneous medium since this was the quantity that was measured experimentally.

$$
\alpha = \frac{2\omega}{c} \text{Im} \sqrt{\varepsilon_m \mu_m}
$$

$$
\approx \frac{2\omega}{c} \text{Im} \left( \sqrt{\varepsilon_h \mu_h} \sqrt{1 + 4\pi \sum f_k (\gamma_k + \beta_k)} \right)
$$

$$
\alpha = \frac{2\omega}{c} \text{Im} \left( N_h \sqrt{1 + 4\pi \sum f_k (\gamma_k + \beta_k)} \right)
$$
Expanding the square root and using

$$\frac{2\omega}{c} \text{Im} \ N_h = \alpha_h \quad (87)$$

$$\alpha = \alpha_h + 4\pi \frac{\omega}{c} \text{Im} \left( N_h \sum_k (\gamma_k + \beta_k) \right) \quad (88)$$

For low filling fractions, the absorption is the sum of the contributions due to the electric and magnetic polarizabilities of each type of inclusion in addition to the absorption of the host.

C. Models for Powder Samples

At this point, most of the formalism for determining the electromagnetic properties of an inhomogeneous system has already been introduced. The electromagnetic properties of the samples that were studied experimentally were calculated using several models of these samples. In these models, the system was taken to consist of isolated, conducting grains dispersed inside an insulating host. The MGT was used to calculate the properties of this mixture. The grains were in some cases will be viewed as solid metal particles. While in other cases they were assumed to be made up of smaller solid metal particles in electrical contact with each other.
The motivation for including this second category of models comes from scanning electron micrographs of the experimental samples. These micrographs showed that there was a distinct tendency for the solid metal particles to aggregate into larger clusters. The organization of this section is as follows: (1) the solid metal particle picture will be discussed; (2) the clustered metal particle picture will be discussed; (3) the effects of particle and cluster size distributions will then be considered.

Since the absorption coefficient was the quantity that was measured experimentally, the absorption coefficients predicted by these theoretical models were compared with each other and the experimental results. In these comparisons, as in the earlier discussion of the polarizabilities, the Drude model (equation 51) was used to calculate the dielectric function of the metal. For simplicity, a metal particle-vacuum mixture was considered. A particle diameter of 0.14 μM, a cluster diameter of 13.5 μM, and a filling fraction of 0.005 was used as representative of the samples on which the optical measurements were made. It was somewhat difficult to estimate the low temperature electrical conductivity of the individual particles since the degree of
disorder due to dislocations as well as the effects due to the small diameters are unknown. For these calculations, a value of the conductivity 50 times that of the bulk, room temperature value was arbitrarily chosen.

1) Solid Metal Particle Models

The absorption coefficient predicted by one model of a metal powder-vacuum mixture is shown in Figure 14. The absorption coefficient has been normalized by dividing it by the overall metal filling fraction. For this figure, the polarizabilities were calculated using the Mie theory expressions. The absorption coefficient initially increases rapidly with increasing frequency but saturates at about 25 cm\(^{-1}\). A model using the quasi-static electric and Landau and Lifshitz magnetic polarizabilities yields identical results. Both of the models in this category predict normalized absorption coefficients that are over an order of magnitude smaller than those observed experimentally.
Figure 14. Normalized absorption coefficient versus wavenumber for 0.14 μm diameter palladium spheres using the solid particle models and 50 times the room temperature, bulk conductivity
2) **Clustered Particle Models**

When calculating the properties of a system of metal grains which are themselves made up of smaller, solid particles, it is necessary to know the conductivity of the individual clusters. It is not clear whether the EMA or a metal host version of the MGT will produce more accurate results. In Figure 15, the normalized absorption coefficients predicted by two different models are shown. In one model, the conductivity of the cluster were calculated with the EMA. The properties of the cluster-vacuum system were calculated with the MGT and the polarizabilities obtained from the Mie theory. The other model is identical to the first except that the conductivity of the cluster was calculated using the MGT in the reverse of its usual form. That is, when the conductivity of the clusters were calculated, the metal was assumed to be the host. The two models predict very similar results. The absorption coefficient uses rapidly with increasing frequency until it reaches a plateau at about 5 cm\(^{-1}\). The absorption remains fairly constant until it reaches about 25 cm\(^{-1}\) where it increases rapidly in approximately a parabolic form. The absorption coefficient
Figure 15. Normalized absorption coefficient versus wavenumber for 13 µm diameter palladium clusters with a metal filling fraction within the clusters of 0.34 and a metal conductivity of 50 times the room temperature, bulk value.

Curve A: EMA cluster conductivity; Mie theory cluster polarizabilities

B: Reversed MGT cluster conductivity; Mie theory cluster polarizabilities

C: EMA cluster conductivity; simple theories' cluster polarizabilities

D: Reversed MGT cluster conductivity; simple theories' cluster polarizabilities
has both the same shape and about the same magnitude as that observed experimentally. The model which uses the EMA to obtain the conductivity of the clusters predicts a slightly higher absorption than the model which uses the reversed MGT. This is an artifact of the cluster filling fraction, 0.34 (just above percolation) that was chosen when the figure was made. At high cluster filling fractions, the two models yield identical results. If the cluster filling fraction is reduced from a high value of say 0.6 while both the cluster size and the overall metal filling fraction in the system are held constant, the absorption initially increases. This increase occurs because the filling fraction of clusters in the system increases and because the polarizabilities of the clusters increase due to the reduced cluster conductivity. The absorption coefficient of the model which uses the EMA to calculate the cluster conductivity increases more rapidly than that of its MGT analogue until the EMA model's percolation threshold of 1/3 is reached. For cluster filling fractions below 1/3, the EMA model's absorption is reduced drastically due to the drastic reduction in the magnitude of the eddy currents in the cluster. In contrast, the absorption of the MGT model continues to increase.
At a cluster filling fraction of 0.16, the MGT model's absorption coefficient is about twice the value it was at a cluster filling fraction of 0.34 while the EMA model's absorption has been reduced by over an order of magnitude. This difference is shown in Figure 16.

For comparison purposes, the absorption coefficients predicted by two additional models have also been included in Figure 15. These models differ from the first pair in that the simple polarization theories were used to calculate the polarization of the clusters instead of those derived from the Mie theory. The absorption coefficients predicted by these simple models agree quite well with their Mie theory counterparts at low frequencies. At higher frequencies, however, the absorption coefficients predicted by the models using the simple polarizability theories remain at their low, plateau values. They therefore predict absorption coefficients which have the wrong frequency dependence and which are too small at high frequencies compared to those obtained experimentally.
Figure 16. Normalized absorption coefficient versus wavenumber for 13 μm diameter palladium clusters with a metal filling fraction within the clusters of 0.16 and a metal conductivity of 50 times the room temperature, bulk value

Curve A: Reversed MGT cluster conductivity; Mie theory cluster polarizabilities

B: EMA cluster conductivity; Mie theory cluster polarizabilities

C: Reversed MGT cluster conductivity; simple theories' cluster polarizabilities

D: EMA cluster conductivity; simple theories' cluster polarizabilities
3) **Effects of the Particle and Cluster Size Distributions**

In any real sample, many different sizes of particles or clusters of particles are present. Since the Mie theory polarizabilities depend explicitly on the sphere diameters, the absorption coefficient of the collection of spheres will be affected by the presence of many sphere diameters. There are two ways for accounting for the presence of many sphere diameters: (a) some sort of average sphere diameter can be calculated before the polarizabilities are calculated; (b) the polarization of the sample can be obtained by summing the contributions of each particle size.

a) **Volume Averaged Particle Diameter**

In the formalism that has been discussed earlier, the concentration was expressed in terms of the volume filling fraction. When calculating a particle or cluster diameter to represent all of the particles or clusters in a sample, it is important to account for the increase in volume that occurs when the diameter of a sphere is increased. This may be done by calculating a volume averaged sphere diameter, $D_{vw}$.
where \( p_k \) is the probability that a sphere has the \( k^{th} \) diameter, \( d_k \), and \( V_k \) is the volume of the \( k^{th} \) diameter sphere. The summations run over the sphere diameters. Experimentally, the scanning electron microscope reveals that the diameters of both the particles and the clusters can be described by a log-normal distribution. Because this distribution is skewed toward larger sizes, the volume weighted particle diameter is somewhat larger than the medium particle diameter. As an example, the volume weighted diameter is a 1.5 times the medium diameter for many of the samples studied here, while the volume weighted cluster diameter can be up to five times larger than the median cluster diameter.

b) Summation of Contributions of Different Diameters

The contribution of each particle or cluster diameter can be accounted for by treating each sphere diameter as a separate component in the mixture even if all of the spheres are composed of the same material.
In this case, the summation in the MGT expressions for the dielectric function and the magnetic permeability run over all of the sphere diameters. When calculating the volume filling fraction $f_k$ of the $k^{th}$ diameter sphere, it is important to note that the volume of a sphere increases as the cube of the sphere diameter.

$$f_k = f \frac{p_k d_k^3}{\sum_k p_k d_k^3}$$

(91)

where $f$ is the overall metal filling fraction, $p_k$ is the probability that a sphere has the $k^{th}$ diameter, $d_k$, and the summation runs over all of the sphere diameters.

The absorption coefficient obtained when the MGT and the Mie theory polarizabilities are used to obtain the electromagnetic properties of a system of solid particles with a log-normal size distribution is shown in Figure 17. In this model, the contribution of each particle size's polarizabilities were considered. The volume weighted diameter was $0.14 \mu M$ the geometric standard deviation was 1.5. The contributions from the different particle sizes, each separated from the others by integer multiples of the
Figure 17. Normalized absorption coefficient versus wavenumber for solid palladium spheres with 50 times the room temperature, bulk conductivity and diameters which follow a log-normal distribution.

Curve A: overall normalized absorption coefficient

B: contribution of the 4.0 μm diameter spheres

C: contribution of the 2.8 μm diameter spheres

D: contribution of the 2.0 μm diameter spheres

E: contribution of the 0.68 μm diameter spheres

F: contribution of the 0.38 μm diameter spheres

G: contribution of the 0.058 μm diameter spheres
geometric standard deviation, are also shown. The largest particles with a significant probability of being present in the mixture contributes the most to the absorption. The overall absorption coefficient is somewhat smaller but has about the same frequency dependence as the absorption coefficient obtained using a single volume weighted particle diameter.

The decrease in absorption that occurs when the individual particle sizes contributions are considered occurs because there is a significant probability of very small, very poorly absorbing particles being present in the system.

Figure 18 shows the absorption coefficient of a system of clustered particles predicted by a model which includes the contributions from each cluster size. On performing the numerical calculations, the cluster diameter was taken to be 13.5cm with geometric standard deviation, 1.6. The conductivity of the cluster was calculated using the EMA with a cluster filling fraction of 0.34. Mie theory was used to find the polarizabilities of the cluster. The overall absorption is about double that of the equivalent model which used the volume weighted cluster diameter. The contribution to the absorption by each cluster diameter is also shown. Each line
Figure 18. Normalized absorption coefficient versus wavenumber for clustered palladium spheres with a metal conductivity 50 times the room temperature, bulk value. The clusters have a metal filling fraction of 0.34 and diameters which follow a log-normal distribution.

Curve A: overall normalized absorption coefficient
B: contribution of the 37 μm clusters
C: contribution of the 20 μm clusters
D: contribution of the 10 μm clusters
E: contribution of the 5.4 μm clusters
F: contribution of the 2.8 μm clusters
G: contribution of the 0.16 μm clusters
represents absorption due to a cluster size whose diameter differs from those of the other lines by an integer multiple of the geometric standard deviation of the cluster diameter. The large absorption occurs because there is a significant probability of very large, highly absorbing clusters being present in the inhomogeneous system. Of all the models which have been discussed, the absorption coefficient of this last model is closest to that observed experimentally. In chapter four, the results of least squares fit of this model to experimental data will be presented.
CHAPTER III

EXPERIMENTAL PROCEDURE

This chapter will describe the experimental techniques used in this study. It is organized as follows: A) A general discussion of far-infrared fourier interferometry; B) A description of a lamellar grating interferometer that was constructed especially for this study; C) A discussion of sample preparation and characterization; D) A description of the technique used to introduce hydrogen into the palladium samples.

A. Fourier Transform Spectroscopy

Historically, measurements in the far-infrared have been fraught with difficulties due to a lack of powerful sources of far-infrared radiation. While far-infrared lasers are starting to become useful spectroscopic tools, interferometers presently dominate the field. This section will give a brief description of fourier transform spectroscopy. It is divided into two sections: i) A discussion of the mathematical basis of this technique;
ii) A brief description of the major type of interferometers used in the far-infrared region of the spectrum.

1) Basic Mathematical Formulation

In the two important types of far-infrared interferometers, the Michelson and the Lamellar grating interferometers, the light from a single broad-band source is divided into two beams. Each beam transverses a different path. The two beams are then recombined. Upon recombination, interference takes place. The complex amplitudes of the fields in the recombined beam are equal to the sum of the amplitudes of the fields in the two component beams. The intensity of the final beam depends on both the intensities of the beams and their relative phases. The phase is determined by the path difference in the two interferometer arms. When this path difference is zero, constructive interference takes place and the intensity of the final beam is equal to the intensity of the original, undivided beam. If the path difference is not zero, some of the spectral components interfere constructively while others interfere destructively. Therefore, the intensity of the final beam for nonzero path difference is less than that for zero path difference. If the original beam is
monochromatic, the intensity of the final beam is the sum of the two beam intensities multiplied by a cosinosoidal modulation term. The argument of the cosine is proportional to the path difference and inversely proportional to the wavelength of the radiation. If the original beam is not monochromatic, each frequency contributes to the final intensity, $I(\Delta)$.

$$I(\Delta) = \int_{-\infty}^{\infty} s(\sigma) e^{-i2\pi\sigma \Delta} d\sigma + I(\infty) \quad (91)$$

where $\Delta$ is the path difference, $\sigma$ is the reciprocal of the wavelength of the radiation, and $s(\sigma)$ is the spectral distribution. The constant term $I(\infty)$ is equal to the intensity of the final beam for very large path differences. The spectrum can be obtained by Fourier transforming both sides of equation 91

$$S_\perp(\sigma) = \int_{-\infty}^{\infty} [I(D) - I(\infty)] e^{i2\pi\sigma \Delta} d\Delta \quad (92)$$

The output power of an interferometer is greater than that for a grating monochrometers for two reasons. The presence of all spectral components rather than only one component, the Fellgett advantage, obviously increases the power output. A grating monochromator requires that
a substantial portion of the beam be obscured by a slit. Since an interferometer does not require a slit, the Jacquinot (or e'tendue) advantage, the entire area of the beam is available to the detector. Since the detector noise is the same for both types of instruments, the improved signal to noise ratio enjoyed by interferometers compared to grating monochrometers justifies the more complicated data analysis.

There are three difficulties involved in applying equation 92 to a real interferometer: a) The maximum path difference achievable with real equipment is finite; b) Measurements can be made at only a finite number of path differences; c) It is difficult to determine the exact instrument settings that correspond to zero path difference. These difficulties will each be discussed in turn.

a) Finite maximum path difference

Since a real interferometer can achieve only a finite maximum path difference, the integral in equation 91 must be truncated. This truncation results in distortions in the computed spectrum, $S_t(\sigma)$, compared to the ideal spectrum, $S_i(\sigma)$. Ultimately, the resolution of the instrument is determined by these distortions. High resolution requires that the interferograms, $I(\Delta)$,
include measurements made at large path differences. This truncation can be accounted for formally by re- writing equation 91 as

$$S_t(\sigma) = \int_{-\infty}^{\infty} [I(\Delta) - I(\infty)]A(\Delta)e^{i2\pi\sigma\Delta}d\Delta$$  \hspace{1cm} (93)

where \(A(\Delta)\), an apodization function, is some function which is nonzero only in a finite region where \(\Delta < \Delta_{\text{max}}\). The completed spectrum is related to the ideal spectrum by

$$S_t(\sigma) = S_i(\sigma) \ast a(\sigma)$$  \hspace{1cm} (94)

where \(\ast\) denotes convolution and \(a(\sigma)\), the scanning function is the fourier transform of \(A(\Delta)\).

$$a(\sigma) = \int_{-\infty}^{\infty} A(\Delta)e^{i2\pi\sigma\Delta}d\Delta$$  \hspace{1cm} (95)

The resolution of the computed spectrum is determined by the width of the scanning function. If \(A(\Delta)\) is a boxcar function:

$$A(\Delta) = \begin{cases} 1 & |\Delta| < \Delta_{\text{max}} \\ 0 & \text{otherwise} \end{cases}$$  \hspace{1cm} (96)
\( a(\sigma) \) is a \text{sinc} function

\[
    a(\sigma) = \frac{\sin \frac{2\pi \sigma}{\Delta_{\text{max}}}}{2\pi \sigma \Delta_{\text{max}}}
\]  

(97)

This function has width \( \Delta \sigma \sim \frac{1}{\Delta_{\text{max}}} \) but has large sidelobes away from the origin. The sidelobes distort the spectrum. \(^{41}\) One can eliminate some distortions at the expense of the resolution by using an apodization function which does not vanish suddenly at the maximum path difference. \(^{42}\) Norton and Beer have suggested a family of ess-shaped functions which are particularly useful. The properties of this family of functions are discussed by both Norton and Beer\(^{42}\) and Henry and Tanner.\(^{43}\)

\[ \text{b) Discretely sampled interferograms} \]

Only a finite number of evenly spaced points are measured in the interval where \( A(\Delta) \) is nonzero. The spacing of these points is \( \delta \). The fourier transform is approximated by a Fourier series.

\[
    S_S(\sigma) = \delta \sum_{n=-\infty}^{\infty} [I(n\delta) - I(\infty)]A(n\delta)e^{i2\pi n\delta \sigma}
\]  

(98)
where $S_s(\sigma)$ is the spectrum calculated from this series. $S_s(\sigma)$ is a periodic function of $\sigma$ with a periodicity $\Delta \sigma$ determined by $\delta$

$$\Delta \sigma = \frac{1}{\delta} \quad (99)$$

If the bandwidth of the radiation incident on the detector is greater than the periodicity, $\Delta \sigma$, overlapping (or aliasing) of the calculated spectra will occur. This aliasing will severely distort the calculated spectrum. To eliminate the aliasing the bandwidth of the radiation is adjusted with filters. In the very far infrared, typically, low frequency pass filters are employed although band pass filters could, in principle, be used as well. In the first case, the computed spectra extend to 0 cm$^{-1}$.

c) Errors in the location of zero path difference

It is difficult to determine the exact instrument setting that corresponds to zero path difference. Errors in determining zero path difference introduce into the computed spectrum phase errors which cause tilted baselines and other distortions in the calculated spectrum. Instrument misalignment can introduce other kinds of phase errors. To correct for phase errors, one calculates
\[ S(\sigma) = \delta \sum_{n=-\infty}^{\infty} [I(n\delta) - I(\infty)]A(n\delta)e^{i(2\pi n\delta\sigma + \phi(\sigma))} \] (100)

If the sole source of phase errors is due to errors in the location of zero path difference,

\[ \phi(\sigma) = 2\pi \sigma \epsilon \] (101)

where \( \epsilon \) is the error in the location of zero path difference.

2) Typical interferometers

Two types of interferometers, Lamellar grating and Michelson, are commonly used for interferometry in the far infrared. The basic layout of these instruments will be discussed in turn. A detailed discussion of a particular interferometer, OSU's Lamellar grating interferometer, will follow in the next section.

a) Lamellar Grating Interferometer

In a lamellar grating interferometer, the division of the light from source is accomplished by dividing the wavefront with two interleaved sets of plates called a lamellar grating, shown in cross section in Figure 19. One set of plates is stationary and the other set is moveable. The path difference is twice the groove depth
Figure 19. Light reflecting from a lamellar grating
of the grating. The radiation is collimated and directed toward the lamellar grating with a mirror. The radiation reflected by the grating is focused into a light pipe with another mirror as shown in Figure 20, which is a plain view of the lamellar grating at OSU. Because the grating constant of a lamellar grating is twice the groove width, its diffraction pattern contains only the zeroth and all odd orders of radiation. The amplitude of the zeroth order radiation is 180° out of phase with that diffracted into the higher orders. As the groove depth is varied, energy is switched back and forth between the zeroth and higher diffraction orders. Conservation of energy requires that the sum of the energy in all diffraction orders be equal to the energy of the incident radiation. For 100 percent modulation of the interference pattern, it is necessary to exclude all but the zeroth diffraction order from the detector. The frequency at which the diffraction angle becomes so small that higher order radiation begins to mix with the zeroth order radiation in the exit beam is an effective upper limit on the use of the grating. This frequency is such that

\[ \sigma = \frac{f}{sd} \]  

(102)
Figure 20. Optical plan of the OSU Lamellar grating interferometer
where $f$ is the focal length of the collimating mirrors, $s$ is the width of the aperture of the exit light pipe and $d$ is the grating constant.\textsuperscript{45}

The phase velocity of the light passing between the facets of the grating is changed due to wave guide effects. This change occurs only for the polarization with the electric field parallel to grating long dimension and results in a deviation from a pure cosinosoidal modulation of intensity of the low frequency Fourier components with grating position. A lower limit is therefore placed on frequencies with which a given grating is useful. The onset of this effect\textsuperscript{45} occurs when

$$\sigma \approx \frac{2}{d} \quad (103)$$

A lamellar grating interferometer produces a cosinosoidal modulation of radiation with frequencies between these two limits. Construction considerations usually limit the operating range of lamellar grating interferometer to between about 2 and 100 cm$^{-1}$.

b) Michelson Interferometer

A Michelson interferometer is an alternative instrument for producing a cosinosoidal modulation of monochromatic radiation. In this type of instrument, a
beamsplitter divides the incident beam, while the path difference is varied by moving a mirror. Figure 21 shows the plan of the OSU Michelson interferometer, first described by Sanderson and Scott. The upper limit of this instrument's operating range is determined by the choice of beamsplitter and by difficulties in controlling very small mirror movements. The lower frequency limit is determined by the beamsplitter efficiency which falls off at low frequencies as \( \sin(nd) \) where \( n \) is the index of refraction of the beamsplitter material and \( d \) is its thickness.

B. Construction, Peripheral Equipment and Operation of the OSU Lamellar Grating Interferometer

A far infrared interferometer, a lamellar grating interferometer of the type first constructed by Strong and Vanasse was constructed to aid in the experimental measurements in this dissertation. The description of this instrument is divided into five parts: 1) The construction; 2) The cryostat in which the samples and detector were mounted; 3) The detector electronics; 4) The basic operating procedure; and 5) The analysis of the interferometric data. Aside from operating at in higher frequency range, 40 to 150 cm\(^{-1}\), the Michelson
Figure 21. Optical plan of the OSU Michelson interferometer
interferometer is operated in the same manner as the Lamellar grating instrument.

1) Construction of the OSU Lamellar Grating Interferometer

The general layout of the optical and mechanical components of this instrument is shown in Figure 20. All three subassemblies consisting of: 1) the grating and grating drive; 2) the source, chopper and filter wheel; and 3) the collimating mirrors and their mounts are bolted to a bedplate mounted in a large vacuum tank which originally housed a grating monochrometer. Vibration isolation from the surroundings is provided by nitrogen gas filled bellows. Since the bottom of the vacuum tank is flexible, these bellows and located directly under the legs of the bedplate inside the tank.

The lamellar grating was salvaged from a lamellar grating order separator constructed by Vance. The moveable portion of the grating consists of a piece of stainless steel with nine slots 1.25 x 19 cm in dimension machined through it. It was mounted in an aluminum yoke bolted to a ball bearing slide. The stationary portion of the grating is another block of stainless steel with eight 1.25 x 19 cm grooves machined into it. The stationary grating portion is mounted to a back plate with three stainless steel bolts. The holes in the back of
the grating are a hold-over from its order-separator days. To avoid accidentally marring the optical surfaces which were hand lapped on a surface plate, no new mounting holes were drilled. The pitch of the screw threads (1/4-20) makes the grating adjustment very sensitive. (A differential screw arrangement was considered but never installed.) Due to the location of the mounting holes, none of the grating adjustment axes are parallel to the grating facets.

A micrometer is used to translate the moveable portion of the grating. A stepping motor turns the micrometer 1.8° for each input pulse. Each pulse results in a change in optical path difference, step, of 4.932 μm. The grating is held against the micrometer with a string and counterweight arrangement. A worm gear and selsyn motor are provided to turn the body of the micrometer, allowing the operator to adjust the starting point of each interferogram to a small portion of a step. The backlash in the worm gear is minimized with a leafspring.

A high pressure mercury arc is used as a far infrared source. Since the intensity in the far infrared is proportional to the temperature of the plasma (Wien's law), the lowest input power lamp with an arc large enough to fill the input area of the light pipe was chosen. A higher power lamp would have put an additional load on
the lamp cooling system (a copper water jacket) without significantly increasing the far-infrared output because the arc temperature is approximately the same for all of the available lamps.

The two collimating mirrors were taken from a set of five identical mirrors originally used in a White cell intended for molecular spectroscopy. These mirrors have a square cross section (25 cm on a side), a focal length of 50 cm, and an effective aperture of F1.8. Light is taken from the source to the focal point of the output mirror to the polyethylene exit window with 1.27 cm I.D. brass light pipe and right angle bends. Brass was chosen rather than the more reflecting copper because of the superior corrosion resistance of brass compared to the more readily available copper.

A chopper and a filter wheel are located between the source and the light pipe to the input mirror. The filter wheel consists of twelve low pass transmission filters mounted in brass sleeves bolted to an aluminum disk. The aluminum disk serves as a heat sink for the filters. A very light touch is necessary to adjust the filter wheel since it is bolted directly to the armature of a selsyn motor: A multibladed aluminum disk turned by a synchronous motor comprises the chopper. The chopping frequency may be varied from 6 to 500 Hz by changing
the frequency of motor power supply and the number of chopping blades. Choppers with 2, 3, 4, 5 and 7 blades are available.

Before operation, some preliminary alignment of the optical system and of the grating was necessary. With the mercury arc lighted and a white screen in front of the lamellar grating, the input mirror was adjusted so that the center of its beam coincided with the center of the grating. The input mirror was then focused until the size of the lighted area on the screen was unchanged when the screen was moved along a line from the grating center to the mirror center. This constant size implied that the light incident on the grating was parallel. (Unfortunately, this was not a sensitive test for small focusing errors.) The screen was then removed and a smaller screen placed over the end of the exit light pipe. The output mirror was then adjusted until an image of the end of the input light pipe was focused onto the end of the output light pipe. With the lamellar grating set for about a 1 cm groove depth; a depth micrometer was used to measure the depth at the four corners and at the center and the mounting screws adjusted until the two parts of the grating were parallel to ±0.001 inch (25 μm).

2) Cryostat

The samples and detector were mounted in the cryostat shown in Figure 22. The samples themselves will be des-
Figure 22. The cryostat
cribed in a later section. They were bolted to a brass disk shielded from bubbles in the liquid helium coolant by a brass sample can. A stainless steel rod extending from the brass disk to a knob outside the cryostat was provided to enable the operator to change samples by rotating the disk. The assembly consisting of the samples and the brass disk is called a rotator.

Brass 1.27 in I.D. light pipe was used to bring light from the polyethylene vacuum window past a right angle bend and down to the samples. An additional short piece of light pipe directed the transmitted light through a mylar window into a vacuum can containing a 1.2K pumped helium pot. A brass condensing cone directed the light to a brass cavity containing the doped germanium bolometer detector. The cryostat was mounted in a glass dewar set, which was supported by a steel frame. The clamps fastening this frame to the interferometer were adjustable so that the output window of the interferometer could be aligned with the input window of the cryostat.

3) Detector and data acquisition system

The far-infrared radiation changes the temperature and hence, the resistance of the germanium bolometer. The resistance of the detector chip is an exponential function of the chip temperature.
The detector crystal temperature is affected by many factors, including:

a. Temperature of the helium pot
b. Thermal coupling between the detector crystal and the helium pot
c. Bias current
d. Intensity of the background radiation, which travels down the light pipe with the far-infrared radiation
e. Intensity of the chopped far-infrared radiation.

The radiation is chopped so that the voltage across the chip has both an AC and a DC component when a bias current from a battery is passed through the crystal. The AC component of this voltage is fed to a lock-in amplifier. The reference signal for the lock-in amplifier is generated by the light from a lamp, which is also chopped before being detected by a phototransistor. The DC output of the lock-in amplifier is digitized by an integrating digital voltmeter, and this digital value is punched onto computer cards. The stepping process, integration and punching are all controlled by the digital voltmeter.
4) Typical data-taking session

A typical data-taking session will now be described. The samples were prepared and mounted in the cryostat the night before the session. The sample area of the cryostat was evacuated by a mechanical vacuum pump, flushed with nitrogen gas and reevacuated. This sequence was repeated until the dewar has been flushed four times in order to remove water vapor, carbon dioxide and oxygen from the sample volume. The dewar was then filled with nitrogen gas to an absolute pressure of 650 torr for heat exchange during the cool-down process. One could not use helium exchange gas since it would have compromised the vacuum in the helium dewars by permeating the glass walls. The vacuum insulation space of the helium dewar was similarly flushed and filled with about 0.005 STP liters of nitrogen exchange gas. This amounted to a few torr in the helium dewar insulation vacuum space at room temperature. This gas froze out when the sample space was filled with liquid helium. The liquid nitrogen jacket was then filled, and the cryostat was allowed to cool overnight.

The next morning, the liquid nitrogen jacket was topped up (it usually dropped about 20 percent overnight) and the sample area was evacuated. The sample area was then flushed and purged with gaseous helium gas
to remove any residual nitrogen. The cryostat was then brought to atmospheric pressure with helium gas and filled with liquid helium. Meanwhile, the electronics and mercury arc were allowed to warm up. It was also necessary to run several blank cards through the keypunch to verify that the cards were feeding properly without jamming. The keypunch tended to jam frequently if the blank cards were warped due to humidity changes or from being allowed to remain in the keypunch between data-taking sessions. While the 1.2 K pot was pumping down to its operating temperature, the supply dewar was returned to its storage location and the nitrogen vibration isolation system was filled. Since there was very little weight on the bellows underneath the zero adjust selsyn (see Figure 21), the pressure regulator for this bellows was very sensitive. The regulators used in the vibration isolation system operated by admitting nitrogen gas into the bellows when the pressure fell below a set value and venting excess gas when the pressure was above a second, higher, value. For this particular regulator, the difference between these two values is less than the pressure necessary to raise the bellows from its rest position to its operating position. One had to adjust the regulator so that the lower pressure limit was approximately equal to the
operating pressure. Otherwise, the nitrogen which leaked out of the bellows and connecting plumbing was not re­placed and the bellows collapsed. The bellows were generally filled so that the interferometer and cryostat were raised about 2.5 cm. above their rest position. After the bellows were filled, the cryostat was positioned with the input window of the cryostat lined up with the output window of the interferometer. After this adjustment was made, the two window flanges were taped together to avoid accidental movement. This last adjust­ment had to be done after the vibration isolation system was activated because the cryostat platform would flex when the interferometer was raised.

The filters in the interferometer were next moved into position. It was helpful to peer through the plastic top of the vacuum tank while turning the filter control system. The low temperature filters in the cryostat were next brought into position with the aid of the windows in the dewar set. The rotator was then turned until some signal was indicated on the meter on the lock-in amplifier. The filter positions were then readjusted until this signal was maximized. The position of each sample was marked onto the top of the cryostat while noting the location of maxima in the signal as the rotator was rotated. The remainder of
the adjustments were performed with the rotator in the blank position. The bias current was adjusted by varying the connections to a multitap battery until the highest signal was indicated. The chopper motor drive frequency was varied until the largest signal to noise ratio was obtained. Typical settings for the lock-in amplifier and the integrating digital voltmeter are shown in Table 4.

The grating was then moved until the zero path difference position was identified. This position corresponded to the grating position which produces the maximum signal. The course positioning was performed with the stepping motor and the fine positioning was made with the zero adjust screws. When properly located, the signal one step before the zero path difference location was equal to the signal one step after. If necessary, the grating was adjusted for maximum modulation in the interferogram by adjusting the fixed grating portion mounting screws so that the signal was maximized when the moveable grating portion was positioned at the zero path difference location. The interferometer was next evacuated. The pressure in the tank during a session was typically less than 0.1 torr.

Since the card punch would only punch a five-digit number for each data point, the voltage gain of the
<table>
<thead>
<tr>
<th>Upper Limit of Measured Frequency Range (cm⁻¹)</th>
<th>Infrared Filters</th>
<th>AC Component of Voltage Across Detector (Blank Position on Rotator &amp; Large Path Differences (mv))</th>
<th>RC Time Constant (Sec.)</th>
<th>Integration Time (Sec.)</th>
<th>Maximum Path Difference (µm)</th>
<th>Change in Path Difference per Point (µm)</th>
<th>Number Measured Points</th>
<th>Symbol Used in Figures of Corrected Data</th>
<th>Instrument</th>
</tr>
</thead>
<tbody>
<tr>
<td>26 cm⁻¹</td>
<td>BeO, Lif, Bufz, KBr, Kel, low temp, 6mm fused Quartz (high temp)</td>
<td>0.018</td>
<td>0.125</td>
<td>2</td>
<td>1381.0</td>
<td>86.3</td>
<td>32</td>
<td>⊙ Lamellar grating</td>
<td></td>
</tr>
<tr>
<td>60 cm⁻¹</td>
<td>BeO, Lif, Bufz, KBr, Kel, TeCl to KI (low temp)</td>
<td>0.4</td>
<td>0.125</td>
<td>2</td>
<td>1103.7</td>
<td>37.0</td>
<td>64</td>
<td>⊘ Lamellar grating</td>
<td></td>
</tr>
<tr>
<td>110 cm⁻¹</td>
<td>BeO, LiF, BaF₂, KBr &amp; Kel (low temp)</td>
<td>3.1</td>
<td>0.125</td>
<td>2</td>
<td>1262.6</td>
<td>19.7</td>
<td>128</td>
<td>⊕ Lamellar grating</td>
<td></td>
</tr>
<tr>
<td>180 cm⁻¹</td>
<td>BeO &amp; Lif (low temp) BaF₂ (high temp)</td>
<td>0.75</td>
<td>0.125</td>
<td>2</td>
<td>2915.4</td>
<td>11.4</td>
<td>512</td>
<td>× Michelson</td>
<td></td>
</tr>
</tbody>
</table>
lock-in amplifier had to be set so that the integrated signal had no more than five digits. A program, TOP, to correct for minor overflows is listed in Appendix B.

The grating was then backed up several steps before the scan starting point to take up the backlash in the micrometer lead screw and then returned to the starting point. A reversible digital counter counted the impulses produced by the stepping motor controller to aid in positioning the grating.

Each sample was measured in turn with the lock-in amplifier gain increased for less transparent samples if necessary. Usually four scans were made with each sample and five scans were made with each blank for each bandwidth limiting (cutoff) filter. The measurements with the 26 cm⁻¹ cutoff filter generally differed in that all the scans were made with one sample before proceeding to the next due to the difficulty in changing samples with an almost opaque filter in place. Two-sided scans were measured for all of the optical data taken for this dissertation. The resolution was kept low enough that the interference pattern due to multiple internal reflections inside the sample holder was just not resolved.
5) Data analysis

All of the calculations were performed with an Amdal 470 computer using the Fortran language programs listed in Appendix B. The preliminary calculations which have to be performed with any far-infrared interferometer measurements are described in this section. The more specialized calculations are discussed in Chapter IV.

Each interferogen was apodized with the heaviest of Newton and Beer's \(^{42}\) class of apodization functions.

\[
A(n_s) = 0.09 + 0.5875(1-u^2)^2 + 0.3225(1-u^2)^4 \tag{104}
\]

where \(u = n_s/\Delta_{\text{max}}\) is the fractional distance from the point closest to the zero path difference location. Since the signal decreased as the path difference increased, while the noise remained constant, the signal to noise ration, \(S/N\), decreased as well. Apodization with a function such as the one given above tends to give the higher \(S/N\) points a greater weight than those with a lower \(S/N\). This increased the \(S/N\) of the transform at the expense of a halving of the resolution. The value of \(I(\infty)\) was obtained by averaging the last ten points of each interferogram. The transform itself was performed with a Cooley-Tookey fast Fourier
transform subroutine in the IBM Fortran scientific subroutine package. Each spectrum was phase connected by calculating

$$S(\sigma) = \sqrt{S^*_S(\sigma)S_S(\sigma)} \quad (105)$$

Interferometric data for each sample were usually measured four times. Each interferogram was Fourier transformed to find its spectrum $S_i(\sigma)$ and the average spectrum $S_{Av}(\sigma)$, was then calculated.

$$S_{Av}(\sigma) = \frac{1}{M} \sum_{i=1}^{M} S_i(\sigma) \quad (106)$$

where $M$ was the number of scans taken on the sample.

The standard deviation of each spectral point is

$$\sigma_S(\sigma) = \sqrt{\frac{1}{N-1} \sum_{i=1}^{M} (S_i(\sigma) - S_{Av}(\sigma))^2} \quad (107)$$

The transmission coefficients for each sample were calculated by dividing the average of the spectra taken with that sample by the average of the spectra taken with blank position in the rotator, $S_b(\sigma)$,

$$T(\sigma) = \frac{S_{Av}(\sigma)}{S_b(\sigma)} \quad (108)$$

The standard deviation of the ratio $\sigma_T(\sigma)$ was also calculated
These results were then written onto a disk file, copied onto magnetic tape, and stored. All of these calculations were performed with program OUTGFILE which is listed in Appendix B. This program is a very highly modified version of a program obtained from D.B. Tanner. Notice that this program has options other than those described here. It can also process single-sided interferograms, handle interferograms of varying length, interpolate between spectral points, and calculate other functions in addition to the sample transmission coefficient.

C. Sample Preparation and Characterization

The infrared samples themselves were made of mixtures of metal and alumina powders packed into polyethylene containers. The purpose of the alumina was to insulate the metal particles from each other and so reduce the absorption coefficient of the resulting mixtures to something that was small enough to get a measurable amount of light through. Some samples were made with gas evaporated small particles. This section will be divided into four parts: 1) smoke evaporation;
2) mixture preparation; 3) determination of volume filling fractions; 4) determination of particle and cluster sizes.

1) Smoke evaporation

The method used here for the preparation of metal powders is an inert gas smoke evaporation technique similar to that described by Grangvist and Buhrman,\textsuperscript{52} Doland, O'Neill and Ignatiev,\textsuperscript{53} and Russell.\textsuperscript{54}

The entire procedure was performed in a standard vacuum evaporator shown in Figure 23. The material (Au and Pd) was evaporated from a resistively heated alumina-coated molydenium boat. After initially melting the material to drive off surface impurities and to improve thermal conduction between the material and the boat, the bell-jar was opened and a 13 cm diameter, 18 cm tall glass cylinder was placed around the boat and covered with a glass plate. The bell-jar was then sealed, evacuated to below $10^{-5}$ torr, and filled with a few torr of inert gas. The boat was then heated. The heating current was maintained at a constant value until all of the sample material had evaporated. The bell-jar was then opened and those metal particles which had collected on the glass cylinder and plate were brushed into a glass vial with a small brush. The particles
Figure 23. Evaporator used to make smoke evaporated particles
formed when collisions between the metal and inert gas atoms caused the metal atoms to coagulate.

Several variations of this technique were also tried. For a few batches, a tungsten filament was substituted for the boat. However, the majority of the particles were prepared by evaporating from boats because it was feared that the tungsten would contaminate the particles.

A generally unsuccessful attempt was made to prepare oxide-coated particles by performing the evaporation in an inert gas-oxygen atmosphere. When the oxygen particle pressure was low, an ohmmeter revealed that the particles were conducting. When the oxygen partial pressure was higher, the boat burned in two. For that matter, boats seem to burn in two with distressing regularity when either oxygen partial pressure or total pressure were varied. Some oxide-coated particles were obtained and some preliminary infrared measurements were performed. Unfortunately, the scanning electron microscope, SEM, x-ray analysis which will be discussed shortly revealed that these oxide-coated powders were heavily contaminated with some unknown quantity of molydenium.
The details of each batch of smoke evaporated particles including inert gas type, pressure and heater current are tabulated in Table 5.

2) Mixture preparation

For each sample, the metal and alumina were separately weighted and mixed together by stirring with a stainless steel spatula. Several different metal-alumina proportions were tried. If too little metal was included, preliminary infrared measurements showed that the absorption was due almost entirely to the alumina while if too much metal was included, it was impossible to measure the cluster sizes with the scanning electron microscope. A 10:1 (by weight) proportion of alumina to metal seemed to be the most satisfactory ratio.

Those infrared measurements also revealed that the absorption coefficient of the mixtures was larger in poorly mixed than in well-mixed (15-20 minutes stirring times) samples. Presumably, the stirring effected the cluster size.

The mixtures were packed into polyethylene containers. Polyethylene was chosen because it is fairly transparent in the far-infrared aside for an absorption line at 80 cm$^{-1}$. The absorption coefficient of the polyethylene is shown in Figure 24. The mixtures had
Table 5. Details of evaporations

<table>
<thead>
<tr>
<th>Evaporation Number</th>
<th>Infrared Sample Number</th>
<th>Material</th>
<th>Volume Weighted Diameter (μm)</th>
<th>Heated Current (amps)</th>
<th>Charge (cm³)</th>
<th>Pressure (torr)</th>
<th>Gas #1</th>
<th>Gas #2</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>N.A.</td>
<td>Pd</td>
<td>N.A.</td>
<td>292</td>
<td>0.098</td>
<td>500</td>
<td>Ar 97%</td>
<td>O₂ 3%</td>
<td>Conducting</td>
</tr>
<tr>
<td>2</td>
<td>N.A.</td>
<td>Pd</td>
<td>N.A.</td>
<td>292</td>
<td>0.098</td>
<td>2</td>
<td>Ar 80%</td>
<td>O₂ 20%</td>
<td>Conducting</td>
</tr>
<tr>
<td>3 144.4</td>
<td>Pd</td>
<td>N.A.</td>
<td>N.A.</td>
<td>168</td>
<td>0.049</td>
<td>2</td>
<td>Ar 80%</td>
<td>O₂ 20%</td>
<td>Not conducting</td>
</tr>
<tr>
<td>4</td>
<td>Pd</td>
<td>N.A.</td>
<td>N.A.</td>
<td>168</td>
<td>0.074</td>
<td>10</td>
<td>Ar 80%</td>
<td>O₂ 20%</td>
<td>Burned out boat</td>
</tr>
<tr>
<td>5</td>
<td>Pd</td>
<td>N.A.</td>
<td>N.A.</td>
<td>168</td>
<td>0.074</td>
<td>10</td>
<td>Ar 80%</td>
<td>O₂ 20%</td>
<td>Burned out boat</td>
</tr>
<tr>
<td>6</td>
<td>Pd</td>
<td>N.A.</td>
<td>N.A.</td>
<td>168</td>
<td>0.049</td>
<td>10</td>
<td>Ar 96%</td>
<td>O₂ 4%</td>
<td>Burned out boat</td>
</tr>
<tr>
<td>7</td>
<td>Pd</td>
<td>N.A.</td>
<td>N.A.</td>
<td>168</td>
<td>0.049</td>
<td>10</td>
<td>He 80%</td>
<td>O₂ 20%</td>
<td>Conducting</td>
</tr>
<tr>
<td>8</td>
<td>Pd</td>
<td>N.A.</td>
<td>N.A.</td>
<td>168</td>
<td>0.049</td>
<td>10</td>
<td>Xe 80%</td>
<td>O₂ 20%</td>
<td>Burned out boat</td>
</tr>
<tr>
<td>9</td>
<td>Pd</td>
<td>N.A.</td>
<td>N.A.</td>
<td>168</td>
<td>0.049</td>
<td>1.7</td>
<td>He 80%</td>
<td>O₂ 20%</td>
<td>Conducting</td>
</tr>
<tr>
<td>10</td>
<td>Pd</td>
<td>N.A.</td>
<td>N.A.</td>
<td>168</td>
<td>0.049</td>
<td>10</td>
<td>Xe 80%</td>
<td>O₂ 20%</td>
<td>Damaged boat</td>
</tr>
<tr>
<td>11</td>
<td>147-2</td>
<td>Pd</td>
<td>0.036</td>
<td>N.A.</td>
<td>0.049</td>
<td>2</td>
<td>He 100%</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>12</td>
<td>174-4</td>
<td>Pd</td>
<td>0.062</td>
<td>N.A.</td>
<td>0.049</td>
<td>2</td>
<td>He 100%</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>13</td>
<td>174-5</td>
<td>Pd</td>
<td>0.062</td>
<td>N.A.</td>
<td>0.049</td>
<td>10.5</td>
<td>He 100%</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>14</td>
<td>Pd</td>
<td>N.A.</td>
<td>252</td>
<td>0.049</td>
<td>10.5</td>
<td>He 100%</td>
<td>--</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>15</td>
<td>Pd</td>
<td>N.A.</td>
<td>231</td>
<td>0.049</td>
<td>10</td>
<td>He 100%</td>
<td>--</td>
<td>--</td>
<td>For reference chamber</td>
</tr>
<tr>
<td>16</td>
<td>Pd</td>
<td>N.A.</td>
<td>168</td>
<td>0.098</td>
<td>2</td>
<td>He 100%</td>
<td>--</td>
<td>--</td>
<td>For reference chamber</td>
</tr>
<tr>
<td>17</td>
<td>144-3</td>
<td>Au</td>
<td>N.A.</td>
<td>292</td>
<td>0.049</td>
<td>2</td>
<td>Ar 80%</td>
<td>O₂ 20%</td>
<td>Not conducting</td>
</tr>
<tr>
<td>18</td>
<td>Au</td>
<td>N.A.</td>
<td>N.A.</td>
<td>210</td>
<td>0.049</td>
<td>2</td>
<td>He 100%</td>
<td>--</td>
<td>Conducting</td>
</tr>
<tr>
<td>19</td>
<td>Au</td>
<td>N.A.</td>
<td>0.193</td>
<td>292</td>
<td>0.245</td>
<td>2</td>
<td>He 100%</td>
<td>--</td>
<td>Conducting evaporated in boat</td>
</tr>
<tr>
<td>20</td>
<td>Au</td>
<td>N.A.</td>
<td>210</td>
<td>0.245</td>
<td>2</td>
<td>He 100%</td>
<td>--</td>
<td>--</td>
<td>Temperature too high</td>
</tr>
<tr>
<td>21</td>
<td>Au</td>
<td>N.A.</td>
<td>210</td>
<td>0.245</td>
<td>2</td>
<td>He 100%</td>
<td>--</td>
<td>--</td>
<td>--</td>
</tr>
</tbody>
</table>
Figure 24. Absorption coefficient of high density polyethylene.
to be packed into the containers rather tightly so that they would not settle and leave voids where no sample was present in the beam. Even with tight packing, cracks were found in the packed samples when they were opened following optical measurements at low temperatures. Presumably these appeared when the container expanded upon warming up after the session. Measurements made on the first and second cool-down to liquid helium temperature were consistent with each other, indicating that the cracks closed back up when the samples were recooled.

Some very early measurements were made with sample containers made up of two strips of polyethylene separated by a polyethylene spacer with a hole for the mixture cut into it. These had three disadvantages. First, there was uncertainty in the volume filling fraction of the samples because it was difficult to measure the volume of the samples. Second, these containers were difficult to load since they consisted of many parts. Finally, they tended to leak powder. The sample holders shown in Figure 25, which were prepared by the physics department machine shop, were more uniform, considerably easier to load, and retained the powder securely. They consisted of polyethylene blocks with 1.35 cm diameter cylindrical holes either 0.076 cm or 0.154 cm (two samples
Figure 25. Polyethylene sample container
thicknesses were tried) cut into them. The above dimen-
sions are room temperature values. Polyethylene contracts
about 2.449 percent along a linear dimension upon
cooling to 20K. Obviously, this thermal contraction
must be accounted for when calculating the volume of
the sample containers and the absorption coefficients
of the samples.

3) Determination of volume filling fractions

The volume filling fractions of metal, $f_m$, and
alumina, $f_A$, in the samples were found from the measured
mass and the densities of the constituents of the
mixture.

$$f_m = \frac{M_m}{V \rho_m} \quad (110)$$

and

$$f_A = \frac{M_A}{V \rho_A} \quad (111)$$

where $M_A$ is the mass of the alumina used in the sample,
$M_m$ is the mass of the metal, $V$ is the volume of the
sample container and $\rho_m$ and $\rho_A$ are the densities of
the metal and the alumina respectively. The values
for volume and density should those at 4.2K, the tempera-
ture at which the infrared measurements were performed.
Using the tabulated values for the room temperature densities and the National Bureau of Standards values\textsuperscript{55} for the contraction upon cooling to 20K (close enough to 4.2K) the low temperature values of the densities are given in Table 6,

<table>
<thead>
<tr>
<th>Component</th>
<th>4.2K</th>
<th>300K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Palladium</td>
<td>12.25 g/cm\textsuperscript{3}</td>
<td>12.16 g/cm\textsuperscript{3}</td>
</tr>
<tr>
<td>Gold</td>
<td>19.49 g/cm\textsuperscript{3}</td>
<td>19.30 g/cm\textsuperscript{3}</td>
</tr>
<tr>
<td>Alumina</td>
<td>3.91 g/cm\textsuperscript{3}</td>
<td>3.90 g/cm\textsuperscript{3}</td>
</tr>
</tbody>
</table>

One of the samples contained a silver-palladium alloy (65:35). A crude approximation of the low temperature density of this alloy was obtained by finding a weighted average of the densities of silver and palladium and the palladium thermal contraction. This value for the alloy's density was 11.15 g/cm\textsuperscript{3}.

It was also necessary to account for the expansion of the palladium upon the absorption of hydrogen. According to Lewis,\textsuperscript{57} the lattice constant at 25°C for very low hydrogen concentration ($\alpha_{\text{max}}$, which should be close to the hydrogen free value) is 3.895\textsuperscript{\AA} while
the lattice constant for high hydrogen concentrations \( \beta_{\text{max}} \), which should be close to the saturated value) is \( 4.025 \) \( \text{Å} \). This indicates that a linear dimension of the palladium expands about 3.47 percent upon exposure to hydrogen, giving a density at 4.2K for PdH of 11.16 \( \text{g/cm}^3 \). For simplicity, the expansion of the silver palladium alloy was also taken to be this value.

4) Determination of particle and cluster sizes

The scanning electron microscope (SEM) was used to determine the particle and cluster sizes. This discussion will be divided into three parts: a) scanning electron microscopy and x-ray mapping; b) the SEM sample mounting; c) determination of the particle and cluster diameter distributions.

a) Scanning electron microscopy and x-ray mapping

In a SEM, an electron beam is focused onto the sample. The electrons scattered by the sample plus secondary electrons knocked out of the sample are collected and amplified. This signal is then used to control the intensity of the spot on a CRT screen. The electron beam is swept over the sample in a raster pattern. Simultaneously, the display spot on the CRT is swept in an identical pattern. This is, in some
sense, the opposite of normal visual light microscopy. In an usual microscope, the light from a diffuse source is directed at the specimen and the light scattered by a point on the specimen is focused by the microscope optics. Thus, in a normal microscope, the scattered beam is focused, while in a SEM, the incident beam is focused. 58

The x-ray mapping is done by collecting the x-ray photons emitted by the sample when it is struck by the electron beam. These photons are then used to modulate the intensity of the CRT display spot. The electron beam is swept over the sample and the display spot is swept over the CRT in the same manner as normal scanning electron microscopy. Each dot on the CRT display screen represents one or more x-ray photons depending on the setting of the x-ray detector sensitivity. The x-ray detector can be adjusted so that it is only sensitive to x-ray photons within a narrow energy window, which can be tuned to the x-ray emission lines of particular elements. The CRT display is then a map of the locations of those elements. There are three errors associated with this procedure. First, some of the bremsstrahlung x-ray photons will be in the selected energy range, and will contribute to an overall background. Second, the discrimination of elements whose
x-ray emission lines differ by integral factors is affected by a phenomenon called pulse pile up which occurs when two or more x-ray photons enter the detector at about the same time and are treated by the detector as a single photon with an energy equal to the sum of the individual photon energies. Pulse pile up effects the discrimination of palladium atoms from aluminum since the principal palladium emission lines have energies that are about twice those of aluminum (see Table 7). This effect obviously becomes more important if the palladium to aluminum volume ratio is low. Finally, the sample geometry (sometimes referred to as specimen topography) can cause a shadowing effect which may shield some of the x-ray photons from the detector.  

The SEM used in this study was a steroscan 410 manufactured by Cambridge/IMANCO Instrument Company of Cambridge, England owned by The Ohio State University Geology-Mineralogy department. The x-ray mapping was done with a 6200 Multichannel Analyzer and a 7000 Si(Li) x-ray detector manufactured by Ortec Incorporated, division of EG&G of Oak Ridge, Tennessee. The x-ray detector used a lithium drifted silicon crystal operated at liquid nitrogen temperature. The detector resolution, full width at half maximum, was 155eV.
Table 7

X-ray emission lines used for SEM x-ray mapping

<table>
<thead>
<tr>
<th>Element</th>
<th>Line</th>
<th>Energy (KeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Palladium</td>
<td>Lα1</td>
<td>2.838</td>
</tr>
<tr>
<td></td>
<td>Lα2</td>
<td>2.833</td>
</tr>
<tr>
<td></td>
<td>Lβ1</td>
<td>2.990</td>
</tr>
<tr>
<td>Aluminum</td>
<td>Kα1</td>
<td>1.487</td>
</tr>
<tr>
<td></td>
<td>Kα2</td>
<td>1.486</td>
</tr>
<tr>
<td>Silver</td>
<td>Lα1</td>
<td>2.984</td>
</tr>
<tr>
<td></td>
<td>Lα2</td>
<td>2.978</td>
</tr>
<tr>
<td>Gold</td>
<td>Lα1</td>
<td>9.711</td>
</tr>
<tr>
<td></td>
<td>Lα2</td>
<td>9.625</td>
</tr>
<tr>
<td></td>
<td>Mα1</td>
<td>2.123</td>
</tr>
<tr>
<td></td>
<td>Mβ2</td>
<td>2.205</td>
</tr>
<tr>
<td>Molydenium</td>
<td>Lα1</td>
<td>2.293</td>
</tr>
<tr>
<td></td>
<td>Lα2</td>
<td>2.290</td>
</tr>
<tr>
<td></td>
<td>Kα1</td>
<td>17.478</td>
</tr>
<tr>
<td></td>
<td>Kα2</td>
<td>17.373</td>
</tr>
</tbody>
</table>
b) SEM Sample Mounting

The majority of the SEM micrographs were taken of samples packed into holes milled into the standard aluminum stubs. This mounting technique closely approximated the mounting technique used when the infrared measurements were performed. An initial trial of using double-sticky tape proved unsuccessful. If the specimen is not electrically grounded, it will build up a charge which will repel the incoming electrons. It is customary to overcoat nonconducting samples with a conductor such as carbon or gold. This overcoat adds an appreciable thickness that has to be compensated for when size measurements are performed. For powder samples, the overcoat serves the additional function of holding the individual grains in position. Otherwise, they will be displaced by the electron beam. All of the SEM specimens used in this study were overcoated with 100Å of carbon followed by 100Å of gold except those specimens which contained gold particles. The specimens which contained gold powder were overcoated with 200Å of carbon. The overcoating was performed with an evaporation technique by the OSU Department of Geology and Mineralogy SEM operator, Jeffrey H. Franklin.
c) Determination of the particle and cluster diameter distributions

A series of micrograph-x-ray map pairs were made of each sample. The x-ray maps were made with the detector tuned to an energy appropriate for the metal in the sample (see Table 7). The magnifications of the first pairs taken of each sample were adjusted until localized concentrations of particles could just be distinguished (see Plates I and II). The magnification was then increased between successive pairs until a single cluster filled the CRT screen (see Plates III and IV). After one individual cluster had been photographed and mapped, the procedure was repeated until another cluster in the same sample had been located, photographed, and mapped. All of the micrographs and x-ray maps were recorded with a Polaroid 545 film holder on Polaroid 55 P/N film.

Using the x-ray maps as a guide, the diameters of the particles and clusters were measured directly from the micrographs with a caliper. From these measurements, the actual sizes were found by dividing the size on the micrograph by the magnification and then subtracting the thickness of the overcoat. From Figures 26 and 27, which show histograms on linear and logarithmic scales respectively of the diameter
Plate I. Scanning electron micrograph of the mixture used in sample 173-3 (500X)

Plate II. Palladium x-ray map of the region shown in Plate I
Plate III. A typical inclusion that was found in the mixture used in sample 173-3 (5000X)

Plate IV. Palladium x-ray map of the region shown in Plate III
Figure 26. Cluster diameter distribution for 173-3 on a Linear Scale
Figure 27. Cluster Diameter Distribution for 173-3 on a Logarithmic Scale
distributions of the clusters in a typical sample, it is apparent that a log-normal distribution is appropriate for describing the cluster sizes. The particle sizes also follow a log-normal distribution.

Most of the measurements were made from low magnification (about x200) micrographs so that a fair number (10 or so) of the largest clusters were visible. Since a system following a log-normal size distribution has many more small members than large members, the diameters of the smallest clusters were usually measured from higher magnification (about x1000) micrographs. The area of the region that was visible in the micrographs varied as the magnification changed. Therefore, the numbers of clusters of each size found from these higher magnification micrographs were weighted with the ratio of the square of the linear magnifications when the averages and the standard deviations of the natural log of the cluster diameters were obtained.

To determine the size distribution accurately, it was necessary to measure all the clusters in a given region. Any collection of dots on the x-ray maps that appeared to have an identifiable outline were considered to be a metal particle cluster. Several errors are inherent in this procedure. Many of the clusters were small. While some of the larger metal clusters were
partially hidden by alumina clusters. Fluctuations in the background noise were undoubtedly identified as clusters. To test the internal consistency of this procedure, a couple of micrographs with the same magnification of different regions of a single sample were measured. This was repeated for a second sample. The results for the median radius agreed to within 30 percent for the two regions. The median diameters, the geometric standard deviations, and the volume weighted diameters are listed in Table 8 for the particles and clusters in each sample.

D. Hydrogenation of Palladium

The motivation for introducing hydrogen into these samples was to change the electrical properties of the metal without changing the geometry of the samples aside for a metal volume increase in PdH of 11 percent. The resulting change in the optical properties of the powder sample provides a severe test for a theoretical description of the optical properties of the sample. This section consists of the properties of the palladium hydride system; and a description of the technique used to introduce hydrogen into the palladium samples.
Table 8. Particle and cluster sizes

<table>
<thead>
<tr>
<th>Material</th>
<th>Median Diameter (μm)</th>
<th>Geometric Standard Deviation</th>
<th>Volume Weighted Diameter (μm)</th>
<th>Median Diameter (μm)</th>
<th>Geometric Standard Deviation</th>
<th>Volume Weighted Diameter (μm)</th>
<th>Alumina</th>
<th>Infrared Sample</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pd (0.036)</td>
<td>0.019</td>
<td>1.5</td>
<td>0.036</td>
<td>11.2</td>
<td>2.1</td>
<td>03.0</td>
<td>B</td>
<td>147-2</td>
</tr>
<tr>
<td>Pd (0.062)</td>
<td>0.022</td>
<td>1.70</td>
<td>0.062</td>
<td>12.9</td>
<td>2.0</td>
<td>07.5</td>
<td>B</td>
<td>149-2</td>
</tr>
<tr>
<td>Pd (0.14)</td>
<td>0.10</td>
<td>1.3</td>
<td>0.14</td>
<td>2.8</td>
<td>1.9</td>
<td>13.0</td>
<td>0.3</td>
<td>173-2</td>
</tr>
<tr>
<td>Pd (0.57)</td>
<td>0.40</td>
<td>1.4</td>
<td>0.57</td>
<td>2.7</td>
<td>2.1</td>
<td>19.0</td>
<td>C</td>
<td>152-5</td>
</tr>
<tr>
<td>Pd (1.9)</td>
<td>0.39</td>
<td>1.9</td>
<td>1.9</td>
<td>2.3</td>
<td>2.0</td>
<td>15.0</td>
<td>C</td>
<td>152-3</td>
</tr>
<tr>
<td>(Ag-Pd) (0.33)</td>
<td>0.13</td>
<td>1.7</td>
<td>0.33</td>
<td>3.4</td>
<td>1.9</td>
<td>18.0</td>
<td>0.3</td>
<td>173-5</td>
</tr>
<tr>
<td>Au (0.19)</td>
<td>0.069</td>
<td>1.7</td>
<td>0.19</td>
<td>11.0</td>
<td>1.7</td>
<td>31.0</td>
<td>B</td>
<td>174-3</td>
</tr>
<tr>
<td>Au (1.3)</td>
<td>0.40</td>
<td>1.7</td>
<td>1.3</td>
<td>2.3</td>
<td>1.9</td>
<td>11.0</td>
<td>C</td>
<td>174-2</td>
</tr>
<tr>
<td>Alumina (C)</td>
<td>0.38</td>
<td>1.4</td>
<td>0.53</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Alumina (B)</td>
<td>0.033</td>
<td>2.5</td>
<td>0.73</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Alumina (0.3)</td>
<td>0.13</td>
<td>2.1</td>
<td>0.95</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
1) The palladium hydride system

The palladium hydride system was first investigated by Graham in 1866. Since then, it has been studied by many workers. A very extensive review of this system is given by Lewis in his book, \textit{The Palladium Hydrogen System}.\footnote{Lewis, \textit{The Palladium Hydrogen System}}

At room temperature, palladium absorbs hydrogen readily while remaining metallic and ductile.\footnote{The diffusion constant is fairly large, \( D = 5 \times 10^{-6} \text{ cm}^2/\text{sec} \).} The hydrogen atoms are absorbed interstically into the octahedral sites in the FCC palladium lattice.\footnote{The diffusion constant decreases exponentially with decreasing temperature, however.} The hydrogen atoms diffuse into the metal after the disassociation of the hydrogen molecules at the metal surface. At room temperature, the diffusion constant is fairly large, \( D = 5 \times 10^{-6} \text{ cm}^2/\text{sec} \).\footnote{It is customary to use the atomic ratio, \( x = \frac{H}{Pd} \), to describe the hydrogen concentration. The hydrogen concentration is a function of both the hydrogen partial pressure and the temperature. At room temperature and a hydrogen partial pressure of one atmosphere, the equilibrium concentration is \( x = 0.6 \). As the pressure is increased or the temperature is decreased, the equilibrium concentration increases to a saturation value of \( x=1 \). At high temperatures or low pressures, the equilibrium}
concentration decreases. The equilibrium concentration is zero at zero hydrogen pressure.\textsuperscript{64}

The electrical properties of the metal change when hydrogen is introduced. These properties are conveniently described by the resistivity ratio,

$$r(x,T) \equiv \frac{\rho(x,T)}{\rho(0,273k)}$$

($\rho(x,T)$ is the electrical resistivity). At room temperature, as the hydrogen concentration is increased from $x=0$, $r(x,273k)$ initially increases. It reaches a maximum of $r=1.7$ at $x=0.6$. It then drops to $r=1$ at $x=1$.

At lower temperatures, the hydrogen concentration dependence of $r(x,T)$ is similar to the room temperature behavior. At 20k, for example, $r(1,20k)=0.1$ while the maximum value of this function is $r=0.79$ at $x=0.74$. Of course, at low temperatures and $x=0$, $r(0,T)$ depends strongly on the purity of the sample.\textsuperscript{65}

Palladium hydride becomes a type II superconductor at $x=0.81$. With increased hydrogen content, the transition temperature rises to $T_c=9k$ at $x=1$.\textsuperscript{66}

2) Hydrogenation technique

Hydrogen was introduced into the samples by filling the sample chamber of the cryostat with hydrogen gas
while the entire apparatus was still at room temperature. The liquid nitrogen jacket of the cryostat was then filled and the samples were allowed to cool. As the temperature fell, the hydrogen content of the samples increased due to the increase in the equilibrium hydrogen concentration. Eventually, the samples cooled to the point where no further change in the hydrogen concentration could occur due to the small value of the low temperature diffusion constant. Since the diffusion constant was small, the sample chamber could then be safely evacuated without degrading the hydrogen concentration of the samples. It was necessary to evacuate the sample chamber before filling it with liquid helium to avoid freezing the hydrogen on the samples and optics. The infrared measurements were then made in the usual manner and compared to those obtained from earlier, hydrogen free measurements.

To determine the hydrogen content, two reference chambers each containing about 200mg of palladium powder were mounted near the infrared samples inside the cryostat sample chamber. These reference chambers, shown in cross section in Figure 28, were made of a copper rod with a 6mm diameter cylindrical cavity drilled about 12mm deep into one end. A 6mm O.D. thin wall stainless steel tubing connected the cavity to a needle value.
Figure 28. Reference chamber for determining the hydrogen concentration within the palladium samples
The needle valves could be closed from outside of the cryostat by stainless steel rods.

After the infrared measurements were performed, the cryostat was permitted to warm up to 77k and evacuated. The valves on the reference chambers were then closed. Next, the reference chambers were removed from the cryostat, attached to a pressure gauge, and heated in paraffin wax to 200°C. The hydrogen concentration was obtained from the quantity of the evolved gas.

\[ x = \frac{H}{pd} = \frac{2n_H}{n_{pd}} \quad (113) \]

where \( n_H \) is the number of moles of molecular hydrogen evolved and \( n_{pd} \) is the number of moles of palladium present in the reference chambers.

\[ n_H = \frac{P}{R} \left( \frac{V_C}{T_C} + \frac{V_g}{T_g} \right) \quad (114) \]

where \( P \) is the absolute pressure in the gauge, \( R \) is the gas constant, \( V_C \) and \( T_C \) are the volume and temperature of the heated portion of the reference chamber respectively, and \( V_g \) and \( T_g \) are the volume and temperature of the remainder of the apparatus.
The needle valves could be closed from outside of the cryostat by stainless steel rods.

After the infrared measurements were performed, the cryostat was permitted to warm up to 77k and evacuated. The valves on the reference chambers were then closed. Next, the reference chambers were removed from the cryostat, attached to a pressure gauge, and heated in paraffin wax to 200°C. The hydrogen concentration was obtained from the quantity of the evolved gas.

\[ x = \frac{H}{pd} = \frac{2n_H}{n_{pd}} \quad (113) \]

where \( n_H \) is the number of moles of molecular hydrogen evolved and \( n_{pd} \) is the number of moles of palladium present in the reference chambers.

\[ n_H = \frac{P}{R} \left( \frac{V_C}{T_C} + \frac{V_g}{T_g} \right) \quad (114) \]

where \( P \) is the absolute pressure in the gauge, \( R \) is the gas constant, \( V_C \) and \( T_g \) are the volume and temperature of the heated portion of the reference chamber respectively, and \( V_g \) and \( T_g \) are the volume and temperature of the remainder of the apparatus.
Before performing the measurement with the infrared samples, some preliminary measurements, with only the reference chambers present in the cryostat, were performed. These preliminary measurements differed from the one involving the infrared samples in that the cryostat was only cooled to 77K instead of down to 4.2K. The results of these preliminary measurements along with the results obtained when the infrared samples were present in the cryostat are given in Table 9. The results for the first preliminary measurement differed from those of the later measurements because the quantity of hydrogen available in the cryostat during this measurement was not sufficient to saturate the entire quantity of palladium. Because the two reference chambers had to compete for the available hydrogen, differences in hydrogen absorption rates were important enough to cause difficulties with this measurement.

For all cases in which enough hydrogen was present to saturate the samples, the results of measurements with each reference chamber were essentially the same. The variations in the results that were present are probably an indication of the uncertainties inherent in this hydrogen concentration measurement technique and the reproducability of this technique.
Table 9. Concentration of hydrogen in the palladium samples

<table>
<thead>
<tr>
<th>Measurement Number</th>
<th>Reference Chamber #1</th>
<th>Reference Chamber #2</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.41</td>
<td>0.22</td>
<td>Not enough H₂ to saturate Pd</td>
</tr>
<tr>
<td>2</td>
<td>0.58</td>
<td>0.78</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.54</td>
<td>0.80</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.56</td>
<td>0.79</td>
<td>Infrared samples also in cryostat</td>
</tr>
</tbody>
</table>
The table does show a discrepancy between the results obtained with each reference chamber. Chamber 2 was filled with commercially prepared palladium powder, Pd(0.14). It packed down into the copper cavity quite nicely so that all of the powder was contained in the copper cavity and none extended into the stainless steel tube joining the cavity to the needle valve. In contrast, the palladium in chamber 1, #15 and #16 in Table 5, did not pack down as well and perhaps 20 percent of it extended into the reference chambers stainless steel tube. Because this stainless steel tube was attached to the needle valve with soft solder having a melting point of 185°C, the tube and the palladium could not be heated to the 200°C outgassing temperature. Consequently, some portion of the palladium in reference chamber 1 retained some of its hydrogen during the heating process so that the hydrogen concentrations for reference chamber 1 inferred from these measurements were lower than the actual concentration. Because all of the palladium in reference chamber 2 was contained within the copper cavity it has been assumed that the palladium inside reference chamber 2 was all heated to the 200°C temperature required to evolve the hydrogen.

The palladium hydride phase diagram indicates that some hydrogen is retained within the metal at 200°C.
This residual concentration of about \( x=0.05 \) must be added to the concentration obtained from equation 109. The concentration of hydrogen within the infrared samples was, therefore, about \( x=0.85 \), the value obtained from the measurements on reference chamber 1. The bulk superconducting transition temperature for this hydrogen concentration is 2.22K which is considerably below the temperature, 4.2K at which the infrared measurements were performed.66
CHAPTER IV

ANALYSIS

The validity of any theory is determined by its ability to accurately predict the experimental measurements to which it is applied. Oftentimes, corrections for systematic errors must be made before an experimental result can be compared to a theoretical prediction. In this chapter, the theoretical models for the far-infrared absorption in small-particle mixtures will be compared to the measurement data by a least-squares fitting procedure.

A. Corrections for Systematic Errors

The systematic difficulties that had to be accounted for before the theory and the experimental data could be compared included the effects of multiple internal reflections in sample or sample holder, absorption by the polyethylene sample holder, the presence of the alumina power, changes or drifts in the detector sensitivity, reflections from the power mixtures, and variations in the concentration of metal between samples.
1) Interference pattern

The frequency dependence of the transmittance of samples whose surfaces are parallel to a fraction of the wavelength has a periodic modulation due to multiple internal reflections. The frequency between adjacent maxima is given by

$$\Delta \sigma = \frac{1}{2t\text{Re}(N)}$$  \hspace{1cm} (115)

where \(t\) is the sample thickness and \(N\) is the index of refraction of the material. The maximum resolution used for the infrared measurements was chosen to be low enough that none of the interference patterns were resolved. Fortunately, these samples had no sharp features so that high resolution measurements were not necessary.

2) Sample holder

Since the effects of multiple internal reflections were avoided, the absorption and reflection due to the sample container could be dealt with by considering only the intensity of the light rather than the complex amplitudes of the component fields. The transmission of the powder samples themselves were obtained by dividing
the transmissions of the polyethylene enclosed powders by the transmission of an empty sample container.

Since some of the samples were exposed to hydrogen gas, measurements were made on an empty sample container both before and after it had been immersed in hydrogen. The absorption coefficients obtained from these two measurements, Figures 24 and 29, were almost identical. The differences that were present were most likely due to the errors inherent in the infrared measurements themselves rather than any change in the sample container.

3) The alumina powder

Mixing the metal and alumina powders yielded a three component, metal-alumina-vacuum mixture rather than the two component, metal-insulator mixture which was discussed in Chapter II. To make a valid comparison, it was necessary to correct for the absorption of the alumina. The low concentration expansion for the absorption coefficient predicted by the MGT (equation 88) showed that the absorption due to the host and the different types of inclusions are separately additive and that the absorption due to each type of inclusion is proportional to its volume filling fraction. The concentrations of the alumina and metal powders in the infrared samples used in this study were all relatively
Figure 29. Absorption coefficient of sample holder after soaking in hydrogen.
low, with volume filling fractions of the metal powders being a factor of 40 smaller than those of the alumina. The data were corrected for the absorption of the alumina by subtracting from absorption coefficients of the mixtures the measured absorption coefficient of the alumina powder after scaling the measured alumina absorption by the ratio of the volume filling fractions of the alumina in the pure alumina and the alumina-metal mixtures.

The absorption coefficient of each of the types of alumina used in mixing the infrared samples is shown in Figures 30 to 32. The absorption coefficient of the alumina increases with increasing frequency. The absorption coefficient of the alumina with the smallest particles is much larger than that of the other alumina samples. Even so, the absorption coefficient of the most absorbing alumina is still small compared to the absorption coefficient of the metal powders. The corrected absorption coefficient of the metal power is given by

$$\alpha = \frac{1}{t_m} \left[ \ln \left( \frac{T_s}{T_h} \right) - \frac{t_m}{t_a} \frac{f_{as}}{f_{aa}} \ln \left( \frac{T_a}{T_h} \right) \right] + \alpha_0 \quad (116)$$

where $t_m$ and $t_a$ are the thicknesses of the samples containing the alumina-metal mixture and the pure alumina respectively, $T_s$, $T_a$ and $T_h$ are transmission coefficients of the alumina-metal filled sample holder, the pure
Figure 30. Absorption coefficient (normalized by dividing by the alumina filling fraction) of alumina C.
Figure 31. Absorption coefficient (normalized by dividing by the alumina filling fraction) of alumina B.
Figure 32. Absorption coefficient (normalized by dividing by the alumina filling fraction) of alumina 0.3.
alumina filled sample holder, and the empty sample holder respectively, and $f_a$ and $f_a^\prime$ are the filling fractions of the alumina in the alumina-metal mixture and pure alumina samples respectively. The additive constant $c_0$ is used to correct for drifts in the detector sensitivity and for reflection from the samples.

4) Detector nonlinearities

Some systematic errors in the measured absorption coefficient were introduced by changes in the detector sensitivity arising from changes in the DC component of the detector temperature which moved the detector to a different position on its resistance versus temperature curve. The DC component of the temperature, in turn, was dependent on the total infrared energy incident on the detector and the heat leak from the detector to the pumped helium pot. Changing either the filters or the samples altered the total energy incident on the detector and hence its temperature. In particular, these changes altered the fraction of the 300k black-body background radiation from the room temperature portion of the cryostat and the interferometer which traveled down the light pipe to the detector. Additional changes in the DC detector temperature occurred when the liquid helium level in the cryostat decreased
because this increased the heat leak to the pumped helium pot and hence the detector from the 4.2K helium bath. This detector sensitivity change corresponded to an additive constant, \( a_0 \), which varied with filter, sample and the level of the 4.2K helium bath. The variations that occurred between different segments of the absorption coefficient that were calculated from data taken with different filters were eliminated by subtracting a constant from each segment so that the low frequency end of one segment would agree with the high frequency and of the segment immediately below it in frequency. To determine the overall correction, an appeal was made to some previously published experimental observations. For completely static fields, one would expect the absorption coefficient to vanish. Since the equipment available for this study was unsuitable for measurements below about 6 cm\(^{-1}\) which corresponds to 180,000 Megahertz, the question of how the absorption coefficient approaches zero immediately arise. Tanner, Sievers and Buhrman\(^6\) and Russell\(^54\) have observed that for low frequencies, the absorption coefficient of metal powders decreases quadratically with decreasing frequency. With this in mind, the overall correction was determined by fitting the experimentally determined absorption coefficient at low frequencies to
\[ \alpha_{\text{exp}} = \alpha_0 + C \sigma^2. \]  

(117)

The value found for \( \alpha_0 \) was subtracted from the data to ensure that it went as

\[ \alpha = C \sigma^2. \]  

(118)

There were two complications inherent in this fitting procedure. The S/N drops sharply at the upper and lower wavenumber ends of each segment. These low S/N portions were eliminated from each segment before the matching and parabolic fitting were performed. The other difficulty involved the portions of the absorption coefficient which did not vary quadratically. While the earlier workers did not find a quadratic behavior at the upper end of the wavenumber range measured here, there was a difficulty with the low wavenumber end as well. What is, a low wavenumber for some cluster sizes is not necessarily a low wavenumber for larger clusters. This effect was illustrated in Chapter II in Figure 18.

To overcome these problems, the parabolic fitting was performed on only those portions of the data that appeared to have a quadratic behavior.
5) Reflection from the sample surfaces

Because of reflection losses at the two surfaces of the samples, the experimentally measured transmittance is equal to

\[ T = \frac{(1-R)^2e^{-\alpha t}}{1-R^2e^{-2\alpha t}} \]  \hspace{1cm} (119)

where \( \alpha \) is the power absorption coefficient of the sample, \( t \) is the sample thickness, and \( R \) is the single surface reflectance,

\[ R = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2} \]  \hspace{1cm} (120)

In this equation, \( n = \text{Re}(N) \) and \( k = \text{Im}(N) \). When the absorption coefficient is calculated from the transmittance, one must account for this reflectance. If \( R^2e^{-2\alpha t} \ll 1 \), the second term in the denominator of equation 117 may be neglected. This equation then yields

\[ \alpha = -\frac{1}{t} \ln T + \frac{2}{t} \ln (1-R) \]  \hspace{1cm} (121)

The second term was partially removed when the parabolic fitting procedure, described in the last section, was used to obtain the overall correction for detector
sensitivity and other drifts. A check on this procedure can be had if the reflection term is calculated for a suitable sample and compared to the corrections that were actually obtained.

The real and imaginary part of the index of refraction are related by the Kramers-Kronig relation:

\[ n - 1 = \frac{P}{\pi} \int_{-\infty}^{\infty} \frac{k}{\omega' - \omega} \, d\omega', \quad (122) \]

where \( P \) denotes the principal part. Taking \( N(-\omega) = N^*(\omega) \) expressing the frequencies in terms of wavenumbers, and expressing \( k \) in terms of the absorption coefficient,

\[ n - 1 = \frac{P}{2\pi^2} \int_{0}^{\infty} \frac{\alpha(\sigma')}{\sigma'^2 - \sigma^2} \, d\sigma', \quad (123) \]

This equation is particularly simple and easy to evaluate at zero frequency, where it gives

\[ n(0) - 1 = \frac{P}{2\pi^2} \int_{0}^{\infty} \frac{\alpha(\sigma')}{\sigma'^2} \, d\sigma'. \quad (124) \]

Sample 149-2 has the largest high frequency absorption coefficient and therefore the metal in this sample is
expected to have the largest contribution to the refractive index. Evaluating the integral in equation 122 using the data for this sample, shown in Figure 36, the zero frequency contribution of the metal to the sample's refractive index is 0.05. The zero frequency refractive index of the entire sample has contributions from the metal, the alumina, and of course, the voids contained in the sample. The effective contribution to the refractive index of a sample containing only the alumina at the volume fraction for this sample can be estimated from the MGT to be 0.07. With no metal, the samples have n=1.07 while with the metal n=1.12. At zero frequency, the contribution of the metal to k is zero since $\alpha = \frac{\omega}{c} k$ and $\alpha$ goes to zero quadratically. The contribution of the alumina is very small at 4.2K, while, of course, the contributions of the voids is zero. The reflection causes an error, $\alpha_R$, in the absorption coefficient calculated from equation 121.

$$\alpha_R = -\frac{2}{t} \ln(1-R)$$  \hspace{1cm} (125)

Therefore, the reflectance of the sample without the metal is 0.0010 while with the metal, R=0.0032. Therefore, $\alpha_x/\omega=15 \text{ cm}^{-1}$ for this sample at zero frequency if the metal had no contribution or $\alpha_x/\omega=45 \text{ cm}^{-1}$ if the contribution of the metal is included. By way of comparison, the parabolic fitting procedure described above returned $\alpha_0/\omega=210 \text{ cm}^{-1}$ which is much larger than the above numbers.
The frequency dependence of $\alpha_r$ is more important than its zero frequency value since the parabolic fitting procedure insured that the experimental absorption coefficient vanished at zero frequency. It is fairly simple to estimate an upper limit on $\alpha_r$ at high frequencies. The contribution of the alumina and the voids to the refractive index of the mixture is essentially constant over the entire frequency range.\(^{69}\) Examination of the Kramers-Kronig relation, equation 122, shows that the maximum value of $N-1$ for the metal occurs at zero frequencies. Using this value as an upper limit on the high frequency value of $N-1$ and the value of $k$ obtained from the high frequency absorption coefficient,

$$k = \frac{\alpha}{4\pi\sigma} = 0.033,$$  \hfill (126)

an upper limit on the high frequency reflectance is 0.0035. This corresponds to $\alpha_r/f = 48$ which is only 0.3 percent of the high frequency absorption coefficient. More importantly, the difference between the high frequency and zero frequency values of $\alpha_r/f$ is only 0.02 percent of the normalized high frequency absorption coefficient. The frequency dependence of the reflection therefore has a negligible effect on the measured absorption coefficient.
6) The metal volume fraction

To compare the absorption of different samples, it was necessary to account for the effects due to differences in concentration which occurred when the sample containers were filled. The experimental absorption coefficients were normalized by dividing by the volume filling fraction of the metal. While the theoretical, low concentration expression for the absorption coefficient is proportional to the metal volume filling fraction, this normalization did not eliminate all of the differences between samples due to concentration because the environment of the metal powders depended on the concentration of alumina in the samples. It was still possible to compare different samples, however, because the alumina-metal volume ratios were about the same for all of the samples. The results were not affected by any errors in the measurement of the sample thickness because the logarithms of the sample transmission coefficients were divided by the product of the thickness and the volume filling fraction. This product is independent of thickness,

\[ ft = \frac{m}{\rho A} \]  \hspace{1cm} (127)

where \( m \) is the mass of metal, \( \rho \) the metal density, and \( A \) the cross-sectional areas of the sample.
The corrected data and the fitted parabolic lines are shown in Figures 33-53. The values of C from equation 118 are given in Table 10. For the majority of the samples, the parabolas fit the data quite well over most of the frequency range. There were some discrepancies, however. For many samples, for frequencies less than about 30 cm\(^{-1}\), the data tended to be above the line that fitted the majority of the data points, while for high frequencies, the data tended to drop below this parabolic line. Samples 173-2 and 174-2 did not seem to fit a parabola very well. These last two samples may have contained some very large clusters that absorbed heavily at low (< 30 cm\(^{-1}\)) frequencies, but saturated at higher frequencies.

B. Fit of Theory to Experiment

After the corrections described above were made, the absorption coefficients of some of the samples were fit to the theoretical model by a least-square process. The theoretical model used for this fitting was the one that used the EMA to obtain the conductivity of the clusters, the Mie theory results for the polarizabilities of the clusters, and which included a log-normal distribution for the cluster diameters. For samples without hydrogen, both the filling fraction
Table 10. Results of parabolic fitting procedure

<table>
<thead>
<tr>
<th>Material</th>
<th>C/f(cm)</th>
<th>Not Hydrogenated</th>
<th>Hydrogenated</th>
<th>Volume Weighted Cluster Diameter (Unhydrogenated) (µm)</th>
<th>Infrared Sample Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pd (0.036)</td>
<td>12.35</td>
<td>2.295</td>
<td>2.036</td>
<td>83.2</td>
<td>147-2</td>
</tr>
<tr>
<td>Pd (0.062)</td>
<td>16.29</td>
<td>Not measured</td>
<td>Not measured</td>
<td>74.9</td>
<td>149-2</td>
</tr>
<tr>
<td>Pd (0.14)</td>
<td>0.7185</td>
<td>Not measured</td>
<td>Impossible to measure</td>
<td>162-3</td>
<td></td>
</tr>
<tr>
<td>Pd (0.57)</td>
<td>0.2205</td>
<td>Not measured</td>
<td>0.3899</td>
<td>15.4</td>
<td>152-3</td>
</tr>
<tr>
<td>Pd (1.9)</td>
<td>0.2160</td>
<td>Not measured</td>
<td>0.2002</td>
<td>15.1</td>
<td>152-3</td>
</tr>
<tr>
<td>(AG-Pd) (0.33)</td>
<td>0.6087</td>
<td>Not measured</td>
<td>Impossible to measure</td>
<td>162-5</td>
<td></td>
</tr>
<tr>
<td>Au (0.19)</td>
<td>1.610</td>
<td>Not measured</td>
<td>Opaque</td>
<td>220.6</td>
<td>174-3</td>
</tr>
<tr>
<td>Au (1.3)</td>
<td>0.1172</td>
<td>Not measured</td>
<td>Opaque</td>
<td>30.7</td>
<td>174-2</td>
</tr>
<tr>
<td>Oxidized Pd</td>
<td>0.1097</td>
<td>Opaque</td>
<td>Not applicable</td>
<td>144-4</td>
<td></td>
</tr>
<tr>
<td>Oxidized Gold</td>
<td>0.3089</td>
<td>Opaque</td>
<td>Not applicable</td>
<td>144-3</td>
<td></td>
</tr>
</tbody>
</table>
Figure 33. Normalized, corrected absorption coefficient for sample 147-2, Pd(0.0036), versus wavenumber. The fitted parabolic line is also shown.
Figure 34. Normalized, corrected absorption coefficient for sample 174-4, Pd(0.036), versus wavenumber. The fitted parabolic line is also shown.
Figure 35. Normalized, corrected absorption coefficient for sample 174-4 with hydrogen, Pd H$_{0.036}$ versus wavenumber. The fitted parabolic line is also shown.
Figure 36. Normalized, corrected absorption coefficient for sample 149-2, Pd(0.062), versus wavenumber. The fitted parabolic line is also shown.
Figure 37. Normalized, corrected absorption coefficient for sample 174-5, Pd(0.062), versus wavenumber. The fitted parabolic line is also shown.
Figure 38. Normalized, corrected absorption coefficient for sample 174-5, Pd(0.062), versus wavenumber. The fitted parabolic line is also shown.
Figure 39. Normalized, corrected absorption coefficient for sample 162-4, Pd(0.14), versus wavenumber. The fitted parabolic line is also shown.
Figure 40. Normalized, corrected absorption coefficient for sample 173-2, Pd(0.14), versus wavenumber. The fitted parabolic line is also shown.
Figure 41. Normalized, corrected absorption coefficient for sample 173-2 with hydrogen, Pd H$_{0.8}$ (0.14), versus wavenumber. The fitted parabolic line is also shown.
Figure 42. Normalized, corrected absorption coefficient for sample 156-5, Pd(0.57), versus wavenumber. The fitted parabolic line is also shown.
Figure 43. Normalized, corrected absorption coefficient for sample 173-4, Pd(0.57), versus wavenumber. The fitted parabolic line is also shown.
Figure 44. Normalized, corrected absorption coefficient for sample 173-4 with hydrogen, Pd H₉₀₈(0.57), versus wavenumber. The fitted parabolic line is also shown.
Figure 45. Normalized, corrected absorption coefficient for sample 156-3, Pd(1.9), versus wavenumber. The fitted parabolic line is also shown.
Figure 46. Normalized, corrected absorption coefficient for sample 173-3, Pd(1.9), versus wavenumber. The fitted parabolic line is also shown.
Figure 47. Normalized, corrected absorption coefficient for sample 173-3 with hydrogen, Pd H$_{0.8}$(1.9), versus wavenumber. The fitted parabolic line is also shown.
Figure 48. Normalized, corrected absorption coefficient for sample 162-5, (AG-Pd)(0.33), versus wavenumber. The fitted parabolic line is also shown.
Figure 49. Normalized, corrected absorption coefficient for sample 173-5, (AG-Pd)(0.33), versus wavenumber. The fitted parabolic line is also shown.
Figure 50. Normalized, corrected absorption coefficient for sample 174-3, Au(0.19), versus wavenumber. The fitted parabolic line is also shown.
Figure 51. Normalized, corrected absorption coefficient for sample 174-2, Au(1.3), versus wavenumber. The fitted parabolic line is also shown.
Figure 52. Normalized, corrected absorption coefficient for sample 144-3, oxidized gold, versus wavenumber. The fitted parabolic line is also shown.
Figure 53. Normalized, corrected absorption coefficient for sample 144-4, oxidized palladium, versus wavenumber. The fitted parabolic line is also shown.
of the metal within the clusters, $F_c$, and the conductivity of the metal were used as fitting parameters. For samples with hydrogen, $F_c$ was held at its pre-hydrogen value while only the conductivity of the metal was varied.

The actual fitting was accomplished with a non-linear least-squares fitting subroutine described by Bevington. This subroutine optimized the fitting parameters by varying them (initial values were provided) until $\chi^2$, the sum of the squares of the deviations of the experimental data from the theoretical function, was minimized.

$$\chi^2 = \frac{1}{\nu} \sum_{j=1}^{N} \frac{(\alpha_T(x_j) - \alpha_j)^2}{\sigma_j^2}$$  \hspace{1cm} (128)

$$\nu = N - n$$  \hspace{1cm} (129)

where $N$ is the number of data points, $n$ is the number of variable parameters, $\alpha_T(x)$ is the theoretical absorption coefficient, $\alpha_j$ is the $j^{th}$ experimental point at frequency $x_j$, and $\sigma_j$ is the standard deviation of the $j^{th}$ experimental point.

The fitted theoretical parameters and $\chi^2_\nu$ for all of the samples are given in Table 11. The corrected
Table 11. Results of the least-square fitting of the theory to the experimental data

<table>
<thead>
<tr>
<th>Sample</th>
<th>Material</th>
<th>$F_c$</th>
<th>$\tau$ (sec)</th>
<th>$\rho$ ($\mu\Omega$-cm)</th>
<th>$r = \frac{\rho(0,4.2k)}{\rho(0,293k)}$</th>
<th>$\chi^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Without Hydrogen</td>
<td>With Hydrogen</td>
<td>Without Hydrogen</td>
<td>With Hydrogen</td>
</tr>
<tr>
<td>173-2</td>
<td>Pd (0.14)</td>
<td>0.41</td>
<td>$0.21 \times 10^{-14}$</td>
<td>$0.27 \times 10^{-15}$</td>
<td>67.64</td>
<td>514.1</td>
</tr>
<tr>
<td>173-4</td>
<td>Pd (0.57)</td>
<td>0.41</td>
<td>$0.22 \times 10^{-16}$</td>
<td>$0.10 \times 10^{-16}$</td>
<td>6394</td>
<td>13437</td>
</tr>
<tr>
<td>173-3</td>
<td>Pd (1.9)</td>
<td>0.41</td>
<td>$0.19 \times 10^{-13}$</td>
<td>$0.12 \times 10^{-14}$</td>
<td>7.506</td>
<td>120.3</td>
</tr>
<tr>
<td>173-5</td>
<td>(AG-Pd) (0.33)</td>
<td>0.36</td>
<td>$0.40 \times 10^{-16}$</td>
<td>---</td>
<td>3.489</td>
<td>---</td>
</tr>
<tr>
<td>174-2</td>
<td>Au (1.3)</td>
<td>0.37</td>
<td>$0.26 \times 10^{-13}$</td>
<td>---</td>
<td>1.685</td>
<td>---</td>
</tr>
</tbody>
</table>

* $r = \frac{\rho(0,4.2k)_{AG-Pd}}{\rho(0,293k)_{Pd}}$
data and the fitted theoretical curves are shown in Figures 54-61. While there are no hard-and-fast rules, it is customary to regard a fit as satisfactory if \( \chi^2_v \) is close to 1 (that is, if \( \chi^2_v < 1.5 \)) since the probability of a random set of points fitting the theoretical function better than the experimental data points is then less than approximately 0.5. Using this criterion and the values of \( \chi^2_v \) for each fitted sample, all of the fits except the one to the data from the hydrogenated sample 173-4 were satisfactory. Examination of the plot of the fitted theoretical function and the experimental data for this sample showed that the fitted theoretical function did appear to follow the experimental data points fairly well. The data from the unhydrogenated samples yielded lower values of \( \chi^2_v \) than their hydrogenated counterparts.

It was possible to perform this least-squares fitting procedure on most of the samples. However, certain of the samples were judged to be unsuitable for fitting. For some of the samples, including most of the samples made from the smoke evaporated particles, the volume weighted cluster diameters were a significant fraction of the wavelength of the radiation in the alumina-vacuum host material over almost the entire
Figure 54. Normalized, corrected absorption coefficient for sample 173-2, Pd(0.14), versus wavenumber. The fitted theoretical line is also shown.
Figure 55. Normalized, corrected absorption coefficient for sample 173-2 with hydrogen, Pd h_{0.8}(0.14), versus wavenumber. The fitted theoretical line is also shown.
Figure 56. Normalized, corrected absorption coefficient for sample 173-4, Pd(0.57), versus wavenumber. The fitted theoretical line is also shown.
Figure 57. Normalized, corrected absorption coefficient for sample 173-4 with hydrogen, Pd H0.8(0.57), versus wavenumber. The fitted theoretical line is also shown.
Figure 58. Normalized, corrected absorption coefficient for sample 173-3, Pd(1.9), versus wavenumber. The fitted theoretical line is also shown.
Figure 59. Normalized, corrected absorption coefficient for sample 173-3 with hydrogen, Pd H0.8(1.9), versus wavenumber. The fitted theoretical line is also shown.
Figure 60. Normalized, corrected absorption coefficient for sample 173-5 (AG-Pd)(0.33), versus wavenumber. The fitted theoretical line is also shown.
Figure 61. Normalized, corrected absorption coefficient for sample 174-2, Au(1.3) versus wavenumber. The fitted theoretical line is also shown.
frequency range. Therefore, the data from these samples were not fitted to the theory.

It was possible to fit the data over most of the measured frequency range. It was necessary to delete certain frequency regions from the data for some samples. The high frequency data points, where the experimental absorption coefficient became concave downwards, were eliminated because it was felt that these points corresponded to a frequency region where the diameters of the clusters were comparable in size to the wavelength of the radiation in the material surrounding the clusters. The low frequency regions were eliminated because it was felt that the high experimental absorption coefficients at low frequencies were caused by a few very large clusters whose diameters were not accounted for in the log-normal distribution.

The host material for the clusters of metal particles was taken to be an insulating medium with a dielectric function obtained from the MGT model of an alumina-void mixture (vacuum host). The alumina filling fraction of this mixture was equal to the alumina filling fraction of the mixture. For convenience, the dielectric function was taken to be real, with $\varepsilon_1 = 9.61$, since the absorption of the alumina, generally the imaginary
part of the dielectric function, had already been removed from the experimental data as described above.

The Drude model was used to find the dielectric functions and hence the conductivities of the bulk metals. In this model,

\[ \varepsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + \frac{i\omega}{\tau}} \]  

(130)

where \( \omega_p \) is the plasma frequency of the metal, \( \tau \) is the relaxation time, and \( \omega \) is the frequency of the radiation. The relaxation time is related to the static, bulk value of the metal's conductivity, \( \sigma_1 \), by

\[ \tau = \frac{4\pi}{\omega_p} \sigma_1 \]  

(131)

The Drude model works particularly well for gold which has a plasma energy \( \hbar \omega_p = 9.01 \text{eV} \). The room temperature, bulk value for the resistivity, the reciprocal of the conductivity, is 1.51 \( \mu \Omega \cdot \text{cm} \).

The parameters for palladium are not as simply obtained as the parameters for gold. For palladium, the onset of interband transitions occurs for frequencies less than the plasma frequency due to the small size
of palladium's band gap. This small gap complicates the determination the plasma frequency. It is possible to estimate the plasma frequency for palladium from reflection measurements such as those given by Weaver.  

At the plasma frequency, for metals with a wide band gap, the real part of the dielectric function changes from negative to positive and the reflection coefficient for the bulk metal goes from its large, low frequency value to a much lower value at high frequencies. The electrons which become effective due to inner band transitions act to shift this transition in the reflection coefficient to frequencies higher than the plasma frequency. The reflection coefficient for palladium decreases almost linearly from 0.965 at very low frequencies to about 0.819 when $\omega = 1eV$. At this point, the slope of the curve becomes somewhat shallower. By extending this line down to the value of the reflectance at very high frequencies, 0.093, one obtains an estimate of the plasma energy $\omega_p = 5.97eV$. The bulk, room temperature, static value for the resistivity of palladium is 10.6 $\mu\Omega$-cm. Even though the approximations were probably rather crude, the plasma frequencies for the silver-palladium alloy and for the hydrogenated palladium were taken to be equal to the plasma frequency of pure palladium.
CHAPTER V

DISCUSSION

This dissertation has been concerned with the electromagnetic properties of small metal particle mixtures. The quantity that was measured experimentally was the far-infrared absorption coefficient. For the first time, a theoretical model has been able to describe the experimental results. The aggregation of the metal particles into clusters was of fundamental importance in this theoretical description. The scanning electron microscope confirmed the existence of these clusters. The theoretical absorption coefficients were a strong function of the volume weighted cluster diameters. This was verified experimentally as can be seen by comparing the normalized absorption coefficient of sample #147-2, shown in Figure 33 with the normalized absorption coefficient of sample #174-4, shown in Figure 34. When the volume weighted cluster size was increased by a factor of four, the normalized absorption coefficient at 60 cm\(^{-1}\) doubled. The theoretical description required that the cluster be conductors so that eddy currents could circulate through
them. All of the values of cluster filling fractions obtained from the theoretical fitting did correspond to conducting clusters, being above the percolation threshold of 1/3 for the EMA.

In contrast to the cluster diameter, the conductivity of the metal had only a weak effect on the absorption coefficient of the mixture. Figure 62 shows the theoretical absorption coefficient at 60 cm\(^{-1}\) for 0.4 \(\mu\)m Pd (sample #173-3) when the relaxation time and hence the conductivity of the metal is varied. The absorption coefficient barely doubled when the relaxation time decreased by five decades. The theory does predict that the absorption coefficient will increase if the conductivity of the metal is reduced. This was shown experimentally in two ways. First, comparing two samples with approximately the same volume weighted cluster diameters, the 1.3 \(\mu\)m gold particles (sample #174-2) had a lower normalized absorption coefficient than the 0.57 \(\mu\)m palladium particles (sample #173-4), which would be expected to have a lower conductivity. Second, the absorption coefficient of all of the fitted palladium samples increased when hydrogen, which is known to decrease the conductivity of palladium, was added.

One might wonder about the significance that can be attached to the exact values of the conductivities obtained from the least-square fitting procedure. These
Figure 62. Theoretical, normalized absorption coefficient versus the relaxation time of the metal for sample 173-3
values were obviously somewhat larger than those that one would expect for bulk metals at 4.2K. The high intergrain resistance due to the poor electrical contact between individual particles in the clusters probably accounted for these low average values for the conductivities of the metals.

In summary, the experimental far-infrared absorption coefficients of small metal particle mixtures can be described with a theoretical model which accounts for the aggregation of the particles into conducting clusters which follow a log-normal size distribution. The absorption coefficient of the mixture may be increased by either decreasing the average conductivity of the metal or by increasing the volume weighted cluster diameter.
Classical electrodynamics begins with Maxwell's equations. In cgs-gaussian units, they are:

\[ \nabla \cdot \mathbf{B} = 0, \quad (132) \]
\[ \nabla \cdot \mathbf{D} = 4\pi \rho, \quad (133) \]
\[ \nabla \times \mathbf{E} + \frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} = 0, \quad (134) \]

and
\[ \nabla \times \mathbf{H} = \frac{4\pi}{c} \mathbf{j} + \frac{1}{c} \frac{\partial \mathbf{D}}{\partial t}. \quad (135) \]

It is convenient to employ complex fields in Maxwell's equations. The Fourier component of the electric field of frequency, \( \omega \), may be written as

\[ \mathbf{E}(\mathbf{x}, \omega) = E_0(\mathbf{x}) \cos(\omega t + \theta) = \text{Re}[E_0(\mathbf{x}) e^{-i\omega t}], \quad (136) \]

where \( E_0 \) is the field amplitude, \( t \) is the time, and \( \theta \) is a constant (with respect to time) phase factor. The Re on the right hand side can be omitted as long as only the real part of \( \mathbf{E} \) is used at the end of the calculations. \( \mathbf{E}(\mathbf{x}, \omega) \) is coupled to Fourier components of \( \mathbf{H} \), \( \rho \), and \( \mathbf{j} \) having the same frequencies.
It is also convenient to define a complex dielectric function, \( \varepsilon \). The current density \( \mathbf{j} \) and the electric field are coupled via Ohm's law:

\[
\mathbf{j} = \sigma \mathbf{E}, \\
\mathbf{E} = \varepsilon \mathbf{E},
\]

while \( \mathbf{H} = \mu \mathbf{E} \).

where \( \varepsilon \) and \( \sigma \) are considered to be real numbers but \( \mu \) may be complex. Equation 135 can be written using these constitutive relations as

\[
\nabla \times \mathbf{B} = \frac{4\pi}{c} \sigma \mathbf{E} - \frac{i\omega}{c} \varepsilon \mathbf{E}
\]

where the harmonic time dependence of \( \mathbf{E} \) has been used. The quantities displayed and

\[
\mathbf{j} = \sigma \mathbf{E}
\]

can be combined by defining a complex dielectric function

\[
\varepsilon = \varepsilon_1 + \frac{4\pi i \sigma}{i\omega}
\]

or a complex conductivity.
\[
\sigma = \sigma_1 - \frac{i\omega (\varepsilon - 1)}{4\pi} \tag{143}
\]

These two quantities are not independent, so that

\[
\sigma = -\frac{i\omega (\varepsilon - 1)}{4\pi} \tag{144}
\]

Equation 140 then reduces to

\[
\nabla \times \hat{B} = -i\omega \frac{\mu \varepsilon}{c} \hat{E} \tag{145}
\]

The last point to be considered in this appendix is the absorption coefficient, \(\alpha\), for radiation propagating through a conducting, magnetic, dielectric medium. The wave equation can be obtained from Maxwell's equations by first taking the curl of both sides of equation 134.

\[
\nabla \times \left(\nabla \times \hat{E}\right) = -\frac{1}{c} \nabla \times \left(\frac{\partial \hat{B}}{\partial t}\right) \tag{146}
\]

Next, use the relation

\[
\nabla \times \left(\nabla \times \hat{E}\right) = \nabla(\nabla \cdot \hat{E}) - \nabla^2 \hat{E} \tag{147}
\]

and interchange the spatial and temporal derivations on the right hand side.
\[
\vec{\nabla} \cdot (\vec{v} \cdot \vec{E}) - \nabla^2 \vec{E} = \frac{-1}{c} \frac{\partial}{\partial t} (\vec{\nabla} \times \vec{B}) \tag{148}
\]

Assuming \( \rho = 0 \) inside the medium (this is not unreasonable if the medium is a conductor) and using equations 133 and 145, equation reduces to

\[
\nabla^2 \vec{E} = -\frac{\omega^2}{c^2} \mu \varepsilon \vec{E} \tag{149}
\]

The wave equation for the electric field. It is convenient to consider the case where the spatial variations in the field are only in the \( x \) direction. Using the trial solution

\[
\vec{E} = \varepsilon_0 e^{i \frac{\omega}{c} N x} \tag{150}
\]

where \( N \) is the complex refractive index of the medium. Then

\[
\nabla^2 \vec{E} = -\frac{\omega^2}{c^2} N^2 \vec{E} \tag{151}
\]

Equating the RHS of 150 and 151

\[
\frac{\omega^2}{c^2} N^2 \vec{E} = \frac{\omega^2}{c^2} \mu \varepsilon \vec{E} \tag{152}
\]
Since the wave equation is a second order linear differential equation, it has two linearly independent solutions. The sum of these solutions is

$$E = E_0^+ e^{i\omega N x/c} + E_0^- e^{-i\omega N x/c}$$

The boundary conditions determine the values of $E_0^+$ and $E_0^-$. Since $\varepsilon$ and $\mu$ are complex, $N$ is also complex. $N$ can be separated into its real and imaginary parts

$$N = n + ik$$

If $E$ is propagating in the positive $x$ direction,

$$E = E_0^+ e^{i\omega nx/c - \omega/kx} + E_0^- e^{-i\omega nx + \omega/kx}$$

Since $E$ must remain finite at $x = +\omega$, $E_0^-$ must vanish.

$$E = E_0^+ e^{i\omega nx - \omega/kx}$$

$E$ is reduced by a factor of $e^{-1}$ as it propagates through a distance $(\omega/k)^{-1}$. The intensity $I$, the time average
of the power transmitted through a unit area, is

\[
I = \frac{c}{8\pi} \frac{N}{\mu} \mid E \mid^2
\]  

(158)

The absorption coefficient is defined to be $\alpha$ in

\[
I = I_0 e^{-\alpha k}
\]

(159)

where $I_0$ = intensity at $x=0$. By comparing 157, 158 and 159, the following expression for $\alpha$ is obtained

\[
\alpha = \text{Im} \left( \frac{2\omega}{c} \sqrt{\mu_e} \right).
\]

(160)
APPENDIX B
COMPUTER PROGRAMS

This appendix contains the Fortran language computer programs that were used to analyze the infrared data and to calculate the theoretical curves. It is organized as follows:

1) TOP: This program was used to correct mispunched data decks;
2) OUTGFILE: This program fourier transformed the interferometric data and calculated the transmission coefficient of the samples;
3) DEDUCE: This program extracted the normalized absorption coefficients of the metal powders from the transmission coefficients of the samples;
4) FIT: This program corrected the normalized absorption coefficients for dimensional changes in the samples. It then fitted the theoretical absorption coefficient to the experimental data;
5) Plotting subroutines: These subroutines were used to plot the data on the Versatec plotter installed in the OSU computer center. They are based on a subroutine written by D.B. Tanner.
PROGRAM TO CORRECT DIFFICULTIES THAT CAN OCCUR WHILE DATA
CARDS ARE PUNCHED, PRESENTLY UP TO FIVE SIGNIFICANT FIGURES
ARE PUNCHED FOR EACH DATA POINT. IF THE COUNTER SHOULD RECORD
SIX SIGNIFICANT FIGURES, THE MOST SIGNIFICANT FIGURE IS A
ONE. THIS PROGRAM READS IN A DECK, CHECKS FOR UNSUALLY SMALL
NUMBERS (BELOW A NUMBER THAT IS P.D IN), ADDS 100000 TO THOSE
NUMBERS, SUBTRACTS A CONSTANT FROM ALL NUMBERS (TO REDUCE
THEIR SIZE TO ONLY FIVE SIGNIFICANT FIGURES), AND REPUNCHES
THE DECK. THE NUMBER SUBTRACTED IS THE SAME NUMBER THAT IS
USED IN THE CHECKING PROCESS.

DIMENSION IT (W 101), ADENT (15)
10 FORMAT (1615)
20 FORMAT (F15.2, 15A9.1)
30 FORMAT (I1, L5, F9.5, 3F6.4)
40 FORMAT (15 )

READ THE NUMBER TO BE USED IN CHECKING PROCESS.
THE READ FORMAT IS 15.

READ (5, 40) NMIN

READ (5, 40) NSETS

START THE LOOP WHICH PROCESSES EACH RUN.

DO 300 R = 1, NSETS

READ IN HEADER CARDS AND DATA.

READ (5, 20) BUN, (ADENT (K), K = 1, 15)
READ (5, 30) IPD, WP, STEP, GAIN, THICK, ZERO
READ (5, 10) (II (K), K = 1, NP)

CHECK FOR UNSUALLY SMALL (LESS THAN NMIN) POINTS.
ADD 100000 TO THOSE POINTS.
SUBTRACT NMIN FROM ALL POINTS.

DO 130 K = 1, WP
   IF (II (K) - NMIN) 110, 110, 120
   CONTINUE
110   II (K) = II (K) + 100000
120   CONTINUE
   II (K) = II (K) - NMIN
130   CONTINUE

REPUNCH DECK.

WRITE (7, 20) BUN, (ADENT (K), K = 1, 15)
WRITE (7, 30) IPD, WP, STEP, GAIN, THICK, ZERO
WRITE (7, 10) (II (K), K = 1, NP)
300 CONTINUE
STOP
END
2) OUTGFILE

External Reference: RHARM - Fast Fourier transform subroutine in IBM's Fortran scientific subroutine package
C PROGRAM TO TRANSFORM INTERFEROGRAMS
WILL ACCEPT:
TWO-SIDED NONSYMMETRICAL INTERFEROGRAMS
ONE-SIDED SYMMETRICAL INTERFEROGRAMS
VERSATILE PLOTTER ROUTINE.
OUTPUTS K, V, RATIO(K), AND RSD(K) ONTO UNIT 11.

REAL IDENT, IDENT
* REAL %IDENT, %Y(1040), INV(520), S(520),
* PSA(1040), SA(1040), V(1040),
* THETA(1040), PTHETA(1040), PHI(1040), F(1040),
* PATH(1040), LOG(1040), RATIO(1040), ALPH(1040), ALLOG(1040),
* B(2), A(2), IDENT(20), IDENT(20), 18UN(100), RUD(100), FZ(1040),
* ACAV(1040), ACSO(1040), P(10, 1040),
* RSEDEV(1040), RSSEDEV(1040), SBA(1040), SA(1040), SAI(1040)
EQUIVALENCE (I (1040), V (1)), (SA (1), INV (1)), (S (521), S (1))

1 FORMAT (1.10D12)
2 FORMAT (1H9)
3 FORMAT (315)
4 FORMAT (1H6)
5 FORMAT (1H5)
6 FORMAT (1H4)
7 FORMAT (1H3)
8 FORMAT (1H2)
9 FORMAT (1H1)
10 FORMAT (1H0)
11 FORMAT (1H-1)
12 FORMAT (1H-2)
13 FORMAT (1H-3)
14 FORMAT (1H-4)
15 FORMAT (1H-5)

CALL PLOT 10., 0., 1.
WITHES 10 d
DO 901 WTHES=1, WTHESLS
WRITE (6,2)
READ A CARD TO DETERMINE WHAT GRAPHS TO PLOT
LINEAR >0 PLOT LINEAR GRAPHS
>0 DO ROT PLOT LINEAR GRAPHS
LOG >0 PLOT LOG GRAPHS
>0 DO WOT PLOT LOG GRAPHS
<0 TERMINATE EXECUTION
>0 PLOT INTERFEROGRAMS

READ A CARD TO DETERMINE WHAT GRAPHS TO PLOT
LINEAR >0 PLOT LINEAR GRAPHS
=0 DO NOT PLOT LINEAR GRAPHS
LOG >0 PLOT LOG GRAPHS
=0 DO NOT PLOT LOG GRAPHS
INTER>0 PLOT INTERFEROGRAMS

ISP = 0 DO NOT PLOT INTERFEROMETERS
ISP = 1 PLOT SPECTRA
ISP = 2 PLOT SPECTRA

IPHASE = DUMMY VARIABLE

INT = 0 DO NOT PLOT RATIO
INT = 1 PLOT RATIO

IAL = 0 DO NOT PLOT ALPHA
IAL = 1 PLOT ALPHA

JLN, LSY DETERMINES WHAT SYMBOL TO DRAW (SEE IRRPLOT)

THESE PARAMETERS ARE IN SUCCESSIVE ODD NUMBERED COLUMNS

READ(5,1) LINEAR, LOG, INTER, ISP, IPhase, INT, IAL, IALLOG, JLN, LSY
CONTINUE

READ(5,23) IAXIS, VLO, VHI, VLOGLO, VLOGHI
READ(5,23) BATLO, RATHI
READ(5,23) ALPLO, ALPHI
READ(5,23) ALOGLO, ALOGHI

PHASLO = -3.1415
PHASHI = 3.1415

DRIFT = (RATHI - RATHI) / 10.
DELAL = (ALPHI - ALPHI) / 10.
DELLAG = (VLOGHI - VLOGLO) / 10.
DELAIN = (VHI - VLO) / IAXIS
DELLOG = (VLOGHI - VLOGLO) / IAXIS

ALZERO = 0.0

READ INPUT PARAMETERS FOR ENTIRE DATA SET.

HAVE DETERMINES IF INTERFEROMETERS ARE TO BE AVERAGED.

NAVE = 0 => NO AVERAGING.
NAVE = 1 => AVERAGING (BUT NO CORRECTION FOR DETECTOR SENSITIVITY
NAVE = 2 => AVERAGING (WITH CORRECTION FOR DETECTOR SENSITIVITY

IAPOD DETERMINES LEVEL OF APODIZATION. IAPOD = 0 => NO APODIZATION.
IAPOD = 1, 2, 3 => LIGHT, MEDIUM, OR HEAVY APODIZATION.
IAPOD = 4 => TRIANGULAR APODIZATION.

NZERO DETERMINES IF SPECTRUM ZERO LEVEL IS TO BE SUBTRACTED BEFORE
TAKING RATIO. NZERO = 0 => SUBTRACT ZERO LEVEL. NZERO = 1 => DO NOT
SUBTRACT ZERO LEVEL AS COMPUTED BUT RATHER SUBTRACT ZERO AS READ FROM
SECOND INTERFEROMETER HEADER CARD.
C ITHIRD IS A Dummy Variable
C ITANS DETERMINES WHAT TYPE OF DATA IS TO BE TRANSFORMED
C ITANS=0 => NONSYMMETRIC TWO-SIDED INTERFEROGRAMS
C ITANS=1 => SYMMETRIC ONE-SIDED INTERFEROGRAMS
C THESE PARAMETERS ARE IN SUCCESSIVE OLD NUMBERED COLUMNS.
C
C READ (5,1) WAVE, IAPOD, NZERO, ITHIRD, ITANS
C
C*************************************************************************
C HEAD WSETS. THIS IS EQUAL TO THE NUMBER OF GROUPS OF DATA.
C THE SHORTENED NUMBER OF INTERFEROGRAMS IF WAVE=0. THE READ FORMAT
C IS 315.
C READ THE NUMBER OF POINTS TO BE USED IN ONE SIDES OF THE SHORTENED
C INTERFEROGRAMS. IF NSPTS=0 THE FULL LENGTH WILL BE USED.
C READ THE NUMBER OF OUTPUT POINTS. THIS MUST BE A POWER OF TWO.
C THE INTERFEROGRAM WILL BE EXTENDED TO MLPTS WITH ZEROES. IF MLPTS=0,
C NO EXTENSION WILL BE MADE.
C THE READ FORMAT IS 315.
C START BIG LOOP.
C*************************************************************************
C READ (5,3) WSETS, NSPTS, MLPTS
C NDECK=1
C DO 301 N=1, WSETS
C*************************************************************************
C IF (WAVE) 31, 31, 30
C 30 READ (5,3) NDECKS
C 31 CONTINUE
C NDECK=NDECKS
C*************************************************************************
C EACH INTERFEROGRAM MUST HAVE TWO HEADER CARDS.
C THE FIRST HAS A ROW NUMBER (RUN, F6.0) AND AN ALPHANUMERIC LABEL WHICH
C MUST NOT START UNTIL COLUMN 7.
C THE SECOND CONTAINS INPUT PARAMETERS FOR THE INTERFEROGRAM.
C IDP DETERMINES THE TYPE OF DATA
C IDP=0 THE SAMPLE IS A SAMPLE
C IDP=1 THE SAMPLE IS A BACKGROUND
C WP TELLS HOW MANY DATA POINTS TO BE READ. THERE ARE 16 POINTS PER CARD
C WP MUST GET THE HEADER ONTO THE LAST CARD OF THE INTERFEROGRAM.
C STEP IS THE STEP LENGTH IN MICRONS. CURRENTLY:
C 0.00167 IPS FOR LARGE MICHELSON
C 0.0003164 IPS FOR ASYMMETRIC MICHELSON
C 0.000266 IPS FOR LAMELLAR GRATINGS
C THE RATIO IS DIVIDED BY THE FACTOR "GAIN".
C THICK IS THE SAMPLE THICKNESS. THIS IS USED IN CALCULATING THE
C ABSORPTION COEFFICIENT FROM:
C ALPHA=-1.0*THICK*LN (RATIO)
C ZERO WILL BE SUBTRACTED FROM THE COMPUTED SPECTRUM IF NZERO=1.
C READ FORMAT FOR SECOND HEADER IS 11, 15, 9.3P6
C THUS IS IN COL 1, WP ENDS (11) IN COL 6, STEP IS IN COLS 7-15,
C GAIN IN COLS 16-21, THICK IN COLS 22-27, AND ZERO IN COLS 28-33.
C READ THESE AND THE INTERFEROGRAM. PRINT FIRST HEADER CARD.
C*************************************************************************
C DO 1032 N=1, WP
C A Cavaliers (1)=0.0
C 1032 CONTINUE
C IF (NSET-1) 32, 32, 33
C 32 CONTINUE
C READ (5,34) RUN (1), (IDENT (K), K=1, 15)
C WRITE (6, 25) RUN (1), (IDENT (K), K=1, 15)
C READ (5,5) IDP, WP, STEP, GAIN, THICK, ZERO
READ (5, 7) (Y(K), K = 1, NP)
GO TO 33

33 CONTINUE
READ (5, 24) RUN (WSS), (IDENT(K), K = 1, 15)
READ (6, 25) IPK, NP, STEP, GAIN, THICK, ZERO
READ (6, 25) BUN (RSS), (IDENT(K), K = 1, 15)
REAL (5, 7) (Y(K), K = 1, NP)

C WHITE SECOND HEADER CARD AND INTERFEROGRAM

51 CONTINUE
IF (GAIN) 59, 58, 59
58 GAIN = 1.0
59 IF (THICK) 61, 60, 61
60 THICK = 1.0
61 WHITE (6, 6) IPD, NP, STEP, GAIN, THICK
DO 62 K = 1, NP
Y(K) = Y(K)/GAIN
62 CONTINUE
WHITE (6, 6) (Y(K), K = 1, NP)
STEP = STEP/(10000.0)
IN = IN
BPS = 1.0/(IN*STEP*2.0)
CUTOFF = 1.0/(4.0*STEP)

C CALL SUBROUTINE TO TRANSFORM DATA ACCORDING TO ITTRANS.

ITTRANS = ITTRANS + 1
GO TO (90, 95), ITTRANS

90 CONTINUE
CALL TUSDQ (I, PSPTS, WP, IAPOD, ABETA, RES, MLPTS, RUN, IDENT, RUD, IDENT,
TINTER, STEP, JLX, LST, MODCKS, I, V, ZMAI, ZMIN, ME, MHZ, HZMAI, N, S, INV, SA,
7SUM, DEORM)
GO TO 100

95 CONTINUE
CALL ONEDQ (I, PSPTS, NP, IAPOD, ABETA, RES, MLPTS, HUN, IDENT, RUD, IDENT,
TINTER, STEP, JLX, LST, MODCKS, I, V, ZMAI, ZMIN, ME, MHZ, HZMAI, N, S, INV, SA,
7SUM, DEORM)

100 CONTINUE
IF (NAVE .LE. 2) DEORM = 1.
IF (WSS .EQ. 1) RENORM = DEORM
ITTRANS = ITTRANS - 1
MP = N
NP = N

C LOAD ARRAY FOR LOG PLOTS.

DO 158 M = 2, N
VLOG(M) = ALOG10 (Y(M))
158 CONTINUE
VLOG(1) = VLOG(2) - 1.

C FIND NOISE LEVEL AND ZERO LEVEL OF SPECTRUM.

VARA = 0.
JJ = N/16
TN = N/16 + 1
DO 160 K = JJ, N
SAZERO = SAZERO + SA(K)/TN
160 CONTINUE
VARA = 0.
DO 161 K = JJ, N
VARA = VARA + ((SA(K) - SAZERO)**2)/TN

161 CONTINUE
SDA=SUM(VARA)
SDAPC=SDA*10./SUM
RVARA=VARA/SUM
162 WRITE(6,16)ZMAX,ZMIN,ZZERO
GOTO 166
163 WRITE(6,12)ZMAX,ZMIN,ZZERO,ZZERO
165 WRITE(6,13)SDA,SDAPC,RVARA
C
***********************************************************************
C OUTPUT BACKGROUND, AVERAGE SPECTRA, FIND STANDARD DEVIATION OF
C SPECTRA, AND SET BACKGROUND PARAMETERS.
C BEFORE AVERAGE OF SPECTRA IS MADE EACH POINT IS DIVIDED BY THE
C VALUE OF THE BASELINE OF THE INTERFEROGRAM AT WHITE LIGHT.
C AFTER THE AVERAGING IS DONE, THE AVERAGE IS MULTIPLIED BY THE VALUE OF
C THE BASELINE AT WHITE LIGHT OF THE FIRST INTERFEROGRAM IN THE
C SET BEING AVERAGED. THIS IS AN ATTEMPT TO COMPENSATE FOR
C DRIFTING DETECTOR SENSITIVITY.
C***********************************************************************
C IF (HAVE) 1172,1172,1173
1172 CONTINUE
IF (IPD) 1173, 1173, 1176
1173 CONTINUE
WRITE(6,15)
DO 1175 L=1,N
WRITE(6,16)Y(L),SA(L)
1175 CONTINUE
WRITE (6,2)
1176 CONTINUE
DO 173 M=1,W
ACAV(M)=ACV(M)+RENORM*SA(M)/DENORM
TP(NSS,M)=RENORM*SA(M)/DENORM
173 CONTINUE
174 CONTINUE
DO 177 M=1,W
SA(M)=ACAV(M)/NDECK
177 CONTINUE
IF (NDECKS-1) 2184,2184,2180
2180 CONTINUE
DO 2182 L=1,N
DO 2181 K=1,NDECKS
ACSQ(L)=ACSQ(L)+(TEMP-SA(L))*2
2181 CONTINUE
2182 CONTINUE
DO 2183 L=1,N
ACSU(L)=SORT((ACSQ(L)/(INDECK*(INDECK-1.*)))
2183 CONTINUE
2184 CONTINUE
IF (IPD) 1177,1177,180
1177 CONTINUE
DO 179 L=1,W
PSA(L)=SA(L)-ZZERO
BSDEV(L)=ACSO(L)
179 CONTINUE
IF (PSA(L)) 182,181,182
181 PSD(L)=1.0E-12
182 CONTINUE
175 CONTINUE
ZZERO=ZZERO
NDECKS=NDECKS
DO 277 J=1,N
DECT(J)=DECT(J)
277 CONTINUE
IF (HAVE) 201,201,2186
2186 CONTINUE
WRITE(6,18)
```fortran
WRITE (6, 27)
DO 2187 K = 1, N
WRITE (6, 17) V(K)
2187 CONTINUE
WRITE (6, 19)
GO TO 2191
DO 2190 K = 1, 2
WRITE (6, 17) V(K), SA(K), ACSQ(K)
2190 CONTINUE
WRITE (6, 19)
GO TO 201

C********************************************
C CALCULATE RATIO, STANDARD DEVIATIONS OF RATIO, AND ALPHA AND OUTPUT
C T H E M W I T H S PECTRUM.
C********************************************

180 CONTINUE
DO 189 K = 1, N
RATIO(K) = (SA(K) - SZERO) / PSA(K)
DDEV = SA(K) - SZERO
IP (DDEV) = 2186, 2188, 2189
189 CONTINUE
DDEV = 1.0E-12
188 CONTINUE
RATIO(K) = (ACSO(K) / DDEV) ** 2 * (BSDEV(K) / PSA(K)) ** 2
RATIO(K) = (RATIO(K) ** 2 * RSDEV(K)
BSDEV(K) = SORT (BSDEV(K))
IP (RATIO(K)) = 183, 183, 184
183 CONTINUE
ALPHA(K) = 0.0
GO TO 185
184 CONTINUE
ALPHA(K) = (-1. / THICK) * ALOG (RATIO(K))
185 CONTINUE
ALPHA(K) = ALPHALPHA(K) = ALPHALPHA(K)
GO TO 186
186 CONTINUE
ALPHA(K) = ALOG10 (ALPHA(K))
187 CONTINUE
ALPHA(K) = LOG (ALPHA(K))
GO TO 188
188 CONTINUE
IF (NAVE.EQ.2) HBITE (6, 20)
189 CONTINUE

190 CONTINUE
WRITE (6, 18)
IF (NAVE.EQ.2) WRITE (6, 19)
WRITE (6, 17) V(K), SA(K), ACSQ(K), RATIO(K), RSDEV(K), ALPHA(K),
193 CONTINUE
WRITE (6, 2)

C********************************************
C OUTPUT RATIO(K), AND RSDEV(K) INTO UNIT 11.
C********************************************

196 CONTINUE
WRITE (11, 25) (ALOG(K), IDENT(K), K = 1, 15)
WRITE (11, 3197) THICK
DO 2197 K = 1, N
WRITE (11, 3197) K, V(K), RATIO(K), RSDEV(K)
2197 CONTINUE
FORMAT (15, 5X, 3(1E15.7, 5X))
GO TO 199
196 CONTINUE
WRITE (6, 20)
GO TO 197
197 CONTINUE
WRITE (6, 21)
199 CONTINUE
201 CONTINUE
IF (ISP) 220, 220, 200

C********************************************
C PLOT SPECTRUM.
C********************************************
```
C 200 CONTINUE
A(1) = ZMAX
A(2) = 0.0
CALL IRPLOT (A, 10.0, 2, SALO, DELS)
CALL IRPLOT (SA, SALO, DELSA, VLO, DELLIN, XAXIS, MP,
* INTENSITY, 9, FREQUENCY (CM-1), 16, JLN, LSY,
*RUN, NDECKS, IDENT, NUL, -15, IDENT)
220 IF (IP) 201, 201, 221
221 IF (LINEAR) 240, 240, 230
230 IF (IRA) 234, 233, 231
C PLOT RATIO.
C
C 231 CONTINUE
CALL IRPLOT (RATIO, RATLO, DELR, V, VLO, DELLIN, XAXIS, MP,
* RATIO, 5, FREQUENCY (CM-1), 16, JLN, LSY,
*RUN, NDECKS, IDENT, NUD, NDEWS, JDENT)
233 IF (LINEAR) 241, 241, 232
C PLOT ABSORPTION COEFFICIENT.
C
C 234 CONTINUE
CALL IRPLOT (ALPHA, ALPLO, DELALP, V, VLO, DELLIN, XAXIS, MP,
* ALPHA (CM-1), 12, FREQUENCY (CM-1), 16, JLN, LSY,
*RUN, NDECKS, IDENT, NUD, NDEWS, JDENT)
236 IF (I ALOG) 239, 239, 237
C PLOT LOG OF ABSORPTION COEFFICIENT.
C
C 237 CONTINUE
CALL IRPLOT (ALLOG, ALOGLO, DELALG, V, VLO, DELLIN, XAXIS, MP,
* 1Og10 ALPHA, 14, FREQUENCY (CM-1), 16, JLN, LSY,
*RUN, NDECKS, IDENT, NUD, NDEWS, JDENT)
239 IF (LOG) 249, 249, 240
240 IF (IRA) 243, 243, 241
C PLOT RATIO.
C
C 241 CONTINUE
CALL IRPLOT (RATIO, RATLO, DELR, VLOG, DELLLOG, XAXIS, MP,
* RATIO, 5, LOG10 FREQUENCY, 15, JLN, LSY,
*RUN, NDECKS, IDENT, NUD, NDEWS, JDENT)
243 IF (IALOG) 246, 246, 244
C PLOT ABSORPTION COEFFICIENT.
C
C 244 CONTINUE
CALL IRPLOT (ALPHA, ALPLOG, DELALP, VLOG, DELLLOG, XAXIS, MP,
* ALPHA (CM-1), 12, LOG10 FREQUENCY, 15, JLN, LSY,
*RUN, NDECKS, IDENT, NUD, NDEWS, JDENT)
246 IF (I ALOG) 249, 249, 247
CALL IRPLOT (ALLOG, ALOG, DELALG, VLOG, VLOG, DELLOG, XAXIS, MP, *LOG10 ALPHA, 11, *LOG10 FREQUENCY, 15, JLN, LSY, *RUN, NDECKS, IDENT, RUD, NDENTS, JIDENT)

CONTINUE

CONTINUE BIG LOOP

CONTINUE

WRITE (6, 2)

CONTINUE

CALL PLOTE2
STOP
END
SUBROUTINE ONE (Y, WSPTS, MP, IAPOD, ABETA, RES, MPLTS, RDN, IDENT, RUD, 
JUNLT, INTLN, SLP, JL, LSY, NDECKS, I, V, ZMAX, ZMIN, MZ, MAZ, HZMAX, R, S, 
INV, SA, SUM, TAVE)

SUBROUTINE TO CONVERT ONE-SIDED SPECTRA INTO INTERFEROMETER SPECTRA

PARAMETERS

WSPTS - NUMBER OF DATA POINTS TO BE USED (ONE SIDE)
MP - NUMBER OF POINTS OF RAW DATA
IAPOD - TYPE OF APODIZATION
ABETA - DUMMA
RES - RESOLUTION OF SPECTRA
MPLTS - NUMBER OF SPECTRAL POINTS TO BE CALCULATED
RDN - ARRAY OF RUN NUMBERS
IDENT - LABEL OF NUMERATOR
JDENT - LABEL OF DENOMINATOR NUMBERS
JINTER - DETERMINES IF INTERFEROMETERS IS TO BE PLOTTED
SLP - NUMBER OF SPECTRAL POINTS TO BE PLOTTED (SEE IRPLOT)
NDECKS - NUMBER OF POINTS IN RUN
JL, LSY - TYPE OF POINTS TO BE PLOTTED (SEE IRPLOT)
INV - WORK AREA FOR SUBROUTINE RHARM
SA - ARRAY OF SPECTRA (OUTPUT)
SUM - AVERAGE VALUE OF THE END OF THE INTERFEROMETER

REAL IDENT, JDENT
DIMENSION SA (1), Y (1), IDENT (1), JDENT (1), RDN (1), RUD (1), V (1), X (1), 
INV (1), S (1)
9 FORMAT (/12, 27HAPODISLD RESOLUTION (CM-1) = F7.3)
CLEL LOAD NUMBER OF DATA POINTS, MP, IAPOD, ABETA, RES, MPLTS, RDN, IDENT, RUD, JDENT, 
JINTER, SLP, JL, LSY, NDECKS, I, V, ZMAX, ZMIN, MZ, MAZ, HZMAX, R, S, 
INV, SA, SUM, TAVE)

IMP = N
MP = N
DO 135 J = 1, N
   T (J) = Y (2 * J) * IMP
   CONTINUE
   WRITE (6, 9) RES
   XN = N
   DV = 1.001 / (2.0 * STEP * XN)
   ZMAX = 0
   ZMIN = 10000.
   MZ = MP / 12
   HZMAX = 0.
   DO 140 M = 1, N
      V (M) = (XN-1.1) * DV / 2
      IF (M = MZ) 140, 140, 138
      CONTINUE
138 IF (SA (M) = HZMAX) 140, 140, 139
139 CONTINUE
   HZMAX = SA (M)
   HZ2 = M
   CONTINUE
140 DO 150 R = 1, N
      IF (R = MZ) 156, 156, 150
150 IF (SA (M) = 2 * MZ) 154, 154, 153
153 "MAX=SA (M)"
154 IF (SA (M) - ZMIN) 155, 155, 156
155 "ZMIN=SA (M)"
156 CONTINUE
   RETURN
   END
CALL PLOTZ( XMIN,PLOTZ,PLOT1,MP,0.0)

CALL MAKE0(0.0,MAXW-0.0,0.0,PLOTZ)
CALL MAKE1(0.0,7.5,0.0,0.0,PLOTZ)
CALL MAKE2(0.0,10.0,0.0,0.0,PLOTZ)
CALL MAKE3(0.0,10.0,0.0,0.0,PLOTZ)
CALL MAKE4(0.0,5.0,0.0,0.0,PLOTZ)

CALL POINTZ(0.0,0.0,0.0,0.0,PLOTZ)
CALL POINTZ(7.5,0.0,0.0,0.0,PLOTZ)
CALL POINTZ(10.0,0.0,0.0,0.0,PLOTZ)
CALL POINTZ(10.0,5.0,0.0,0.0,PLOTZ)

CALL PLOTZ( XMIN,PLOTZ,PLOT1,MP,0.0)

CALL MAKE0(0.0,MAXW-0.0,0.0,PLOTZ)
CALL MAKE1(0.0,7.5,0.0,0.0,PLOTZ)
CALL MAKE2(0.0,10.0,0.0,0.0,PLOTZ)
CALL MAKE3(0.0,10.0,0.0,0.0,PLOTZ)
CALL MAKE4(0.0,5.0,0.0,0.0,PLOTZ)

CALL POINTZ(0.0,0.0,0.0,0.0,PLOTZ)
CALL POINTZ(7.5,0.0,0.0,0.0,PLOTZ)
CALL POINTZ(10.0,0.0,0.0,0.0,PLOTZ)
CALL POINTZ(10.0,5.0,0.0,0.0,PLOTZ)

CALL PLOTZ( XMIN,PLOTZ,PLOT1,MP,0.0)

CALL MAKE0(0.0,MAXW-0.0,0.0,PLOTZ)
CALL MAKE1(0.0,7.5,0.0,0.0,PLOTZ)
CALL MAKE2(0.0,10.0,0.0,0.0,PLOTZ)
CALL MAKE3(0.0,10.0,0.0,0.0,PLOTZ)
CALL MAKE4(0.0,5.0,0.0,0.0,PLOTZ)

CALL POINTZ(0.0,0.0,0.0,0.0,PLOTZ)
CALL POINTZ(7.5,0.0,0.0,0.0,PLOTZ)
CALL POINTZ(10.0,0.0,0.0,0.0,PLOTZ)
CALL POINTZ(10.0,5.0,0.0,0.0,PLOTZ)
FIND AND SOLVE AVERAGE VALUE OF INTERFEROGRAM.
CALCULATE THE NOISE OF THE INTERFEROGRAM.

**CONTINUE**

YAVE=0.
JJ=NP–NP/8
YN=NP/8–1
DO 55 K=JJ, NP
YAVE=YAVE+T(K)/YN
55 CONTINUE
DO 57 K=1, NP
T(K)=T(K)–YAVE
57 CONTINUE
IN=NP
RES=1./(IN*STEP*2.)
CNPRP=1./(N.*STEP)
SUM=0.
DO 62 K=JJ, NP
SUM=SUM+T(K)*T(K)/YN
62 CONTINUE
SDEV=SQRT(SUM)
SDPCT=SDEV/T(1)*100.
WRITE(6,10) RES
WRITE(6,10) SDPCT, SDEV, YAVE

APODIZE INTERFEROGRAM. SELECT DEGREE OF APODIZATION ACCORDING TO IAPOD.

**CONTINUE**

IAPOD=IAPOD+1
GO TO (123, 122, 121, 120, 119), IAPOD

**TRIANGULAR APODIZATION**

119 DO 118 K=1, NP
IK=K–1
T(K)=T(K)*((1.0–IK/IN)
118 CONTINUE
RES=RES#2.0
GO TO 72

**HEAVY APODIZATION**

120 CO=0.09
CR=0.0
C2=0.5875
C4=0.3225
RES=1.4*RES
GO TO 125

**MEDIUM APODIZATION**

121 CO=0.26
CR=0.154838
C2=0.894838
C4=0.0
RES=1.4*RES
GO TO 125

**WEAK APODIZATION**
C

122 C0=0.548
C1=0.0633
C2=0.5353
C4=0.0
RES=1.2*RES
GO TO 125

C NO APUDATION

C

123 C0=1.0
C1=0.0
C2=0.0
C4=0.0

125 CONTINUE

DO 71 K=1,NP
IX=K
DK=(IX-1)/IN
UPAR=1.0-DK**2
APOD=C0+C1*UPAR+C2*UPAR**2+C4*UPAR**4
Y(K)=Y(K)*APOD

71 CONTINUE

FIND THE POWER OF TWO WHICH IS JUST LARGER THAN NP.
NOTE: NP SHOULD BE LARGER THAN 15
NP=2**ND

MLPTS=NMLPTS
IF(MLPTS.EQ.0)MLPTS=NP
IF(NP.LT.MLPTS)NP=MLPTS
MP=16
NU=4
NP=NP*2
NU=NU+1
GO TO 74

77 CONTINUE
IAPOD=IAPOD-1
WRITE(6,29) IAPOD,CUTOFF

72 CONTINUE

EXTEND INTERFEROGNAN TO NP+1 WITH ZEROES

MM=MIN+1
MM=MP+1
DO 87 K=MM,MM

81 CONTINUE

DOUBLE INTERFEROGNAM ABOUT ITS END.

DO 85 K=1,MP
Y(MM+K)=Y(MM-K)

85 CONTINUE

CALL FOURIER TRANSFORM SUBROUTINE.
The Fourier coefficients are returned in Y(J).
The sine transforms are returned in even numbered locations.
The cosine transforms are returned in odd numbered locations.
CALL RHAP (T, WU, INV, S, IPERR)
RETURN
END
SUBROUTINE TO CONVERT RAW TWO-SIDED INTERFEROGRAMS INTO PHASE-CORRECTED SPECTRA

INPUT: RAW DATA

NSPTS - NUMBER OF DATA POINTS TO BE USED (ONE SIDE)
LP - NUMBER OF POINTS OF RAW DATA
IAPOD - TYPE OF APODIZATION
ABETA - DUMMY
RES - RESOLUTION OF SPECTRA
HLPTS - NUMBER OF SPECTRAL POINTS TO BE CALCULATED
RUN - ARRAY OF RUN NUMBERS
IDENT - LABEL OF NUMERATOR
JIDENT - LABEL OF DENOMINATOR
JN, LSIT - TYPE OF POINTS TO BE PLOTTED (SEE IRPLOT)
NDECKS - NUMBER OF POINTS IN RUN
I - WORK AREA
V - WORK AREA TO STORE PATH DIFFERENCE
ZMAX
ZMIN
HZ
HZMAX
N - NUMBER OF OUTPUT POINTS
S - WORK AREA FOR SUBROUTINE RHARM
INV - WORK AREA FOR SUBROUTINE RHARM
SA - ARRAY OF SPECTRA (OUTPUT)
SUM - ARRAY OF SPECTRA (OUTPUT)
DENORM - VALUE AT WHITE LIGHT OF LINE PASSING THRU THE ENDS OF THE INTERFEROGRAM

REAL IDENT, JIDENT, RES, HLPTS, RUN, IDENT, RUD, JIDENT, INTER, STEP, JN, LSIT, NDECKS, I, V, ZMAX, ZMIN, N, HZ, HZMAX, N, S, INV, SA, SUM, DENORM

SUBROUTINE TWOSSIDY, NSPTS, NP, IAPOD, ABETAD, RES, HLPTS, RUN, IDENT, RUD, JIDENT, INTER, STEP, JN, LSIT, NDECKS, I, V, ZMAX, ZMIN, N, HZ, HZMAX, N, S, INV, SA, SUM, DENORM

DIMENSION SA(1), Y(1), IDENT(1), JIDENT(1), RUN(1), RUD(1), V(1), I(1), INV(1, 150)

CALL LOAD2S(I, NSPTS, NP, IAPOD, ABETA, RES, HLPTS, RUN, IDENT, RUD, JIDENT, INTER, STEP, JN, LSIT, NDECKS, I, V, ZMAX, ZMIN, N, HZ, HZMAX, N, S, INV, SA, SUM, DENORM)

X HP = N
DO 135 J = 1, N
Y(J) = 0.5 * RES
CONTINUE

HZMAX = 0.
DO 140 M = 1, N
SA(M) = SQRT(I(M) * M/M2)
HZ = M
IF (M > HZMAX) HZMAX = M
CONTINUE

HZMAX = SA(N)
HZ2 = N
DO 150 M = 1, N
IF (M > HZ) 160, 140, 139
CONTINUE

HZMAX = SA(N)
HZ2 = N
DO 150 M = 1, N
IF (M > HZ) 156, 156, 150
150 IF (SA (M) - ZMAX) 154, 154, 153
153 ZMAX = SA (M)
154 IF (SA (M) - ZMIN) 155, 155, 156
155 ZMIN = SA (M)
156 CONTINUE
RETURN
END
DO 73 K=1,NP
   T(K)=T(K+KSH)
73 CONTINUE
KF=KF+KSH
75 CONTINUE
IF(NSPTS-MP+KF-1) 77,80,80
77 CONTINUE
MP=KF+NSPTS-1
80 CONTINUE
C***********************************************************************
C FIND THE AVERAGE VALUE AND NOISE OF EACH END OF THE INTEGRAL
C***********************************************************************

YAVB=0.
   DO 82 R=1,10
      YAVB=YAVB*T(R)
82 CONTINUE
   YAVB=YAVB*0.1
SUM=0.0
   DO 83 K=1,10
      SUM=SUM*(T(K)-YAVB)**2
83 CONTINUE
SDEVB=SQRTR(SUM)
SDPCB=SDEVB/TMAX*100.
WRITE(6,10) SDPCB,SDEVB,YAVB,YAVT=0.0
JJ=NF-9
   DO 87 K=JJ,NP
      YAVT=YAVT+T(K)
87 CONTINUE
   YAVT=YAVT*0.1
SUM=0.0
   DO 89 K=JJ,NP
      SUM=SUM*(T(K)-YAVT)**2
89 CONTINUE
S0BT=SQRTR(SUM)
SDIFT=S0BT(SUM)
SDPCF=SDIFT/TMAX*100.
WRITE(6,10) SDPCF,SDIFT,YAVT
C***********************************************************************************
C SUBTRACT A STRAIGHT LINE BETWEEN YAVB AND YAVT.
C***********************************************************************************

XNP=NP
XRF=KF
SLOPE*(YAVT-YAVB)/(XNP-10)
DENOBH=-YAVB*SLOPE*(XRF-XNP)
   DO 92 K=1,NP
      T(K)=T(K)-(DENOM*SLOPE*(XK-XRF))
92 CONTINUE
C***********************************************************************************
C APODIZE INTEGRAL. SELECT DEGREE OF APODIZATION ACCORDING
C TO IAPOD. APODIZE SYMMETRICALLY ABOUT MAX POINT.
C***********************************************************************************

IAPOD=IAPOD+1
   GO TO (115,114,113,112,101),IAPOD
115 CONTINUE
   RES=RES+2.
   UPAR=K-F
   JJ=J-1
   DO 105 K=1,JJ
   105 CONTINUE
HEAVY APODIZATION

112 CONTINUE
CO=0.09
C1=0.0
C2=0.5675
C4=0.3225
RES=1.6*RES
GO TO 117

MEDIUM APODIZATION

113 CONTINUE
CO=0.26
C1=-0.154838
C2=0.894838
C4=0.0
RES=1.4*RES
GO TO 117

WEAK APODIZATION

114 CONTINUE
CO=0.548
C1=-0.0833
C2=0.5353
C4=0.0
RES=1.2*RES
GO TO 117

NO APODIZATION

115 CONTINUE
CO=1.0
C1=0.0
C2=0.0
C4=0.0

117 CONTINUE
JJK=KP+1
KDF=MP-KP+1
KDF=KDF
DO 118 K=JK,MP
UK=K-KP
UK=UK/IDEN
UPAR=1.0-0K**2
APOD=C0+C1*UPAR+C2*UPAR**2+C4*UPAR**4
T(K)+Y(K)*APOD
118 CONTINUE
JJK=KP-1
MP=KP
DO 119 K=1,JK
K=K
UK=1,-XK/XKF
UPAR = 1.

APOD=C04*C1*DPAR+2*C2*DPAR+2*C4*DPAR+2
Y(K) = Y(K) * APOD
119 CONTINUE
120 CONTINUE
IAPOD=IAPOD-1

C DETERMINE IF THE SIDE BEFORE WHITE LIGHT IS LONGER THAN THE
C SIDE AFTER. SET MP EQUAL TO THE LONGER OF THE TWO SIDES
C UNLESS HLPTS IS LONGER. IF MP IS GREATER, SET MP EQUAL TO
C BLPTS.
C
IF (MP-2*KF+1) 121,121,122
121 CONTINUE
MP=KP
GO TO 123
122 CONTINUE
MP=MP+KF
123 CONTINUE
IF (HLPTS-MP) 125,125,124
124 CONTINUE
BP=HLPTS
125 CONTINUE
MP=MPE-1
N2POW=9
126 CONTINUE
IF (HP-HPE) 128,126,127
127 CONTINUE
HPE=BPE*2
N2POW=N2POW+1
GO TO 126
128 CONTINUE
HP=-HPE
XHP=HP

C IF THE SIDE OF THE INTERFEROGRAM BEFORE WHITE LIGHT IS TOO
C SHORT, EXTEND IT TO THE PROPER LENGTH WITH ZEROS.
C REPEAT FOR THE OTHER SIDE.
C
IFIHP-KP) 132,132,129
129 CONTINUE
JJ=HP-KP
DO 130 K=1,NP
T(K)=T(NP-K+1)
130 CONTINUE
NP=NP+JJ
KF=KF+JJ
DO 131 X=1,JJ
Y(K)=0.0
131 CONTINUE
132 CONTINUE
IF (MP-KF+1-MP) 133,135,135
133 CONTINUE
JJ=MP-KF
MP=MP+1
DO 134 X=1,JJ,MP
Y(K)=0.0
134 CONTINUE
135 CONTINUE

C OUTPUT APODIZED, ZERO LEVELLED, AND EXTENDED INTERFEROGRAM
C
WRITE(6,29) WP,IAPOD,CUTOFF
WRITE (6,8) (I (K) ,K = 1,1P)
IF (INTER) 1145, 1145, 1136

C **********************************************************
PLOT INTERFEROGRAM
C **********************************************************

1136 CONTINUE
DO 1138 K=1,NP
IK = K-1
PATHJK(IK) = IK*STEP+2
1138 CONTINUE
YMAX=0.
DO 1139 K=1,NP
IF (T(K) - TMIN) 1140, 1140, 1139
1139 CONTINUE
YMAX=T(K)
1140 CONTINUE
YMIN=0.
DO 1141 K=1,NP
IF (T(K) - TMIN) 1141, 1142, 1142
1141 CONTINUE
YMIN=T(K)
1142 CONTINUE
F(J) = YMAX
K(J) = YMIN
CALL SCALE(K, 10.0, 2, YLO, DELT)
CALL SCALE(JPATH, 10.0, NP, PLO, DELPAT)
* 'SIGNAL' , 'PATH DIFFERENCE (MICRON)' , 24, JLN, LST,
* 'HON', NDECKS, IDENT, FUN, -15, IDENT
1143 CONTINUE
C REVERSE THE SIDE OF THE INTERFEROGRAM BEFORE WHITE LIGHT.
C REPEAT FOR THE OTHER SIDE.
C **********************************************************

JJ=NP/2
DO 1148 K=1,JJ
TEMPI=T(K)
T(K) = Y(NP-K+1)
T(NP-K+1) = TEMPI
1148 CONTINUE
T(NP+1) = 0.0
NP=NP+1
DO 1149 K=1,JJ
TEMPI=Y(KP)
Y(KP) = T(2*NP-K+1)
Y(2*NP-K+1) = TEMPI
1149 CONTINUE
NP=NP
C CALL FOURIER TRANSFORM SUBROUTINE.
C THE FOURIER COEFFICIENTS ARE RETURNED IN T(J).
C THE SINE TRANSFORMS ARE RETURNED IN EVEN NUMBERED LOCATIONS.
C THE COSINE TRANSFORMS ARE RETURNED IN ODD NUMBERED LOCATIONS.
C **********************************************************
CALL RHARM(T, NPOW, INV, 5, IFREQ)
RETURN
END
3) DEDUCE

External Reference: POLFIT - a subroutine intended to fit a polynomial curve to experimental data. It is described fully by P.R. Bevington.
PROGRAM TO CORRECT DATA FOR THE ABSORPTION OF THE PLASTIC SAMPLE.

The absorption of the alumina PVD, and reflection effects. The ratio of the absorption coefficient to the metal filling fraction is then calculated and stored in a file.

PROGRAM CORRECTS FOR REFLECTION AUTOMATICALLY.

DIMENSION \( V(5,520), W(5,520), ASDEV(5,520), SRATIO(5,520), PSRSDCY(5,520), THICK(5), ABENT(16) \)

DIMENSION \( \bar{\alpha}(5,520), AA(6), AA(6), WWV(3000) \)

DIMENSION \( \alpha(5,520), ASALP(5,520), TLT(5), SSDEV(5), SSDEV(5) \)

DIMENSION \( N(5), MLH(5), NH(5), M(5), M(5), ML(5), N(5) \)

DIMENSION \( TSPACE(5), TSPACE(5), TSPACE(5) \)

DIMENSION \( TV(3000), RRATIO(3000), SSDEV(3000), A(6), AM(6), WWV(3000) \)

DIMENSION \( \alpha(5,520), ASALP(5,520), TLT(5), SSDEV(5), SSDEV(5) \)

DIMENSION \( N(5), MLH(5), NH(5), M(5), M(5), ML(5), N(5) \)

DIMENSION \( TSPACE(5), TSPACE(5), TSPACE(5) \)

DIMENSION \( TV(3000), RRATIO(3000), SSDEV(3000), A(6), AM(6), WWV(3000) \)

DIMENSION \( \alpha(5,520), ASALP(5,520), TLT(5), SSDEV(5), SSDEV(5) \)
DO 109 NC=1,NCUT
   IF (ICUT (NC) .EQ.0) GO TO 109
   WRITE (6,2)
   WRITE (6,10) RUN, (ADENT (K), K=1,15)
   WRITE (6,32) MATH (NC), MATH (NC)
   WRITE (6,34) HTH, AMASSA (NC), AMASSM (NC)
   WRITE (6,33) HALU, AREA, DALUR, DRETL, ZERO
   WRITE (6,35)
   NPNC=NP (NC)
   DO 107 K = 1,HP (NC)
   WRITE (6,20) K, V (NC,K) ,RATIO (NC,K) ,RSDEV (NC,K)
   107 CONTINUE
   IF (NPNC .LT.1) GO TO 120
   CONTINUE
109 CONTINUE
   IF (NSS .EQ.1) GO TO 120

DO 117 NC=1,NCUT
   ISCUT (NC)=ICUT (NC)
   IF (ICUT (NC) .EQ.0) GO TO 117
   WPNC=WP (NC)
   DO 115 K = 1,WPNC
      SMATIO (NC,K)=RATIO (NC,K)
      SMATI (NC,K)=SDEV (NC,K)
      115 CONTINUE
   WP (NC)=WP (NC)
   WP (NC)=WP (NC)
   NLS (NC)=WLS (NC)
   NLS (NC)=WLS (NC)
   NLS (NC)=WLS (NC)
   NLS (NC)=WLS (NC)
   117 CONTINUE
   IF (NSS .EQ.1) GO TO 500
   CONTINUE
120 CONTINUE

DO 127 NC=1,NCUT
   IF (ISCUT (NC) .EQ.0) ICUT (NC)=0
   IF (ICUT (NC) .EQ.0) GO TO 127
   IF (NP (NC) LT.1) WP (NC)=WP (NC)
   IF (NP (NC) LT.1) WP (NC)=WP (NC)
   IF (NP (NC) LT.1) WP (NC)=WP (NC)
   IF (NP (NC) LT.1) WP (NC)=WP (NC)
   IF (NP (NC) LT.1) WP (NC)=WP (NC)
   WPNC=WP (NC)
   DO 125 K = 1,WPNC
      IF (RATIO (NC,K) .EQ. (0.01) RATIO (NC,K)=1.E-15
      IF (RATIO (NC,K) .EQ. (0.0) ) RATIO (NC,K)=1.E-15
      SDEV=SDEV (NC,K)/RATIO (NC,K) **2 + (SDEV (NC,K)/RATIO (NC,K) **2
      SDEV=SDEV (NC,K)/RATIO (NC,K) **2 + (SDEV (NC,K)/RATIO (NC,K) **2
      125 CONTINUE
   127 CONTINUE

CALCULATE NATURAL LOGARITHM OF DATA.
DO 131 ICUT = 1, NCUT
   IF (ICUT(NC) .EQ. 0) GO TO 131
   MPNC = NP(NC)
DO 130 K = 1, MPNC
   IF (RATIO(NC, K) - L(0, 0)) RATIO(NC, K) = 1.F-15
   ALPHA(NC, K) = (-1.) * ALOG(RATIO(NC, K))
   BSALP(NC, K) = (-1.) * RSDEV(NC, K)/RATIO(NC, K)
130 CONTINUE
131 CONTINUE
   KA = NA + 1
   IF (NSS .GT. KK) GO TO 140
C LOAD ALUMINA ARRAYS.
C NOTE: IT IS ASSUMED THAT THE SECOND THRU THE (MAL+1)TH SET OF DATA
C ALLOPED TO THE PROGRAM IS THE ALUMINA TRANSMISSION COEFFICIENT.
C
DO 137 ICUT = 1, NCUT
   IAICUT(MALU, NC) = ICUT(NC)
   IF (ICUT(NC) .EQ. 0) GO TO 137
   MPNC = NP(NC)
DO 135 K = 1, MPNC
   ALPHA(MALU, NC, K) = ALPHA(NC, K)/AMASSA(NC)
   ASALP(MALU, NC, K) = ASALP(NC, K)/AMASSA(NC)
135 CONTINUE
   MPA(MALU, NC) = NP(NC)
   MLA(MALU, NC) = NL(NC)
   NHM(MALU, NC) = NH(NC)
   NHPA(MALU, NC) = NHP(NC)
137 CONTINUE
C SUBTRACT A CONSTANT TERM FROM THE ALUMINA ABSORPTION COEFFICIENT
C TO CORRECT FOR REFLECTION EFFECTS.
C
DO 143 ICUT = 1, NCUT
   IF (ICUT(NC) .EQ. 0) GO TO 143
   MPNC = NP(NC)
   CONST = AREA*DALUM/AMASSA(NC)
DO 142 K = 1, MPNC
   MALU(NC, K) = CONST*ALPHA(MC, K) - ZERO
   RSALP(NC, K) = CONST*ASALP(NC, K)
142 CONTINUE
143 CONTINUE
GO TO 154
140 CONTINUE
C CORRECT DATA FOR EFFECTS OF ALUMINA ABSORPTION BY SUBTRACTING
C A BASS WEIGHTED VALUE OF THE LN OF THE PLAIN ALUMINA DATA.
C
DO 147 ICUT = 1, NCUT
   IF (ICUT(MALU, NC) .EQ. 0) ICUT(NC) = 0
   IF (ICUT(NC) .EQ. 0) GO TO 147
   MPNC = NP(NC)
   MLA(MALU, NC) = MLA(NC) / MG(NC)
   MLA(MALU, NC) = MLA(NC) / MG(NC)
   MLA(MALU, NC) = MLA(NC) / MG(NC)
   MLA(MALU, NC) = MLA(NC) / MG(NC)
145 CONTINUE
147 CONTINUE
SUBTRACT A CONSTANT TERM FROM THE ABSORPTION COEFFICIENT
TO CORRECT FOR REFLECTION EFFECTS.
ALSO, NORMALIZE THE ABSORPTION COEFFICIENT.

DO 153 NC=1,NCUT
    IF (ICUT(NC) .EQ. 0) GO TO 153
    NMC=NP(NC)
    CONSTANT=REAL(A/MASS(NC))
    DO 152 K=1,NMC
        ALPHA(NC,K)=REAL(ALPHA(NC,K))
        RSALP(NC,K)=REAL(RSALP(NC,K))
    CONTINUE
153 CONTINUE

DO 154 NC=1,NCUT
    IF (MATCH .NE. 1) GO TO 170

SUBTRACT CONSTANT FROM EACH CUTOFF SUCH THAT THE DATA IS CONTINUOUS FROM ONE CUTOFF TO THE NEXT.

REAL=0
DO 166 NC=1,NCUT
    IF (ICUT(NC) .EQ. 0) GO TO 166
    SCOR=0.
    IF (REAL .EQ. 0 .OR. REAL(NC) .EQ. 0) GO TO 163
    JJ=NC-1
    SIG=V(NC,REAL(NC)) - V(JJ,REAL)
    SIG=SIG
    IF (SIG .GE. 0.0) SIG=SIG
    RR=REAL(NC) + SIG
    SDEM=V(NC,REAL(NC)) - V(NC,RR)
    SLOPE=SLOPE/SDEM
    SCOR=SCOR+ALPHA(JJ,REAL(NC))
    NMC=NP(NC)
    DO 161 K=1,NMC
        ALPHA(NC,K)=ALPHA(NC,K) - SCOR
    CONTINUE
161 CONTINUE
163 CONTINUE

OUTPUT CUTOFF HATCHED DATA

WRITE (6,2)
    IF (REAL .NE. 0 .OR. REAL(NC) .NE. 0) WRITE (6,42) NC,SCOR
WRITE (MATL=REAL(NC))

OUTPUT CUTOFF MATCHED DATA

WRITE (6,23)
    WRITE (6,10) RUN, (ADENT(K), K=1,15)
    WRITE (6,55)
    NMC=NP(NC)
    DO 165 K=1,NMC
        WRITE (6,20) K,V(NC,K),ALPHA(NC,K),RSDEV(NC,K)
    CONTINUE
165 CONTINUE
166 CONTINUE
170 CONTINUE

LOAD ABSORPTION COEFFICIENT INTO FITTING ARRAYS.

NST=1
DO 176 NC=1,NCUT
    IF (ICUT(NC) .LE. 1) GO TO 176
    KST=MM(NC) - ML(NC) + 1
    NEM=NST*KST+1
    ML(NC)=ML(NC)
NHNC = NH(NC)
KK = NST - 1
DO 175 K = NLNC, NHNC
KK = KK + 1
VV(K) = V(NC, K)
BRATIO(K) = ALPHA(NC, K)
RSALP(K) = RSALP(NC, K)
175 CONTINUE
NST = EN + 1
176 CONTINUE

C /* --------------- */
C /* THIS SECTION IS SKIPPED IF IFIT = 1 */
C /* --------------- */
C IF(IFIT.EQ.1) GO TO 2180
DO 2175 K = 1, NEW
VV(K) = VV(K)**2
2175 CONTINUE
CALL POLPIT(VVV, RATIO, BASDEV, MEN, 2, 1, A, CHISQR)
ZERON = A(1)
CPN = A(2)
DO 2177 K = 1, NEW
RATIO(K) = RATIO(K) - ZERON
2177 CONTINUE
DO 2179 NC = 1, NCUT
IF(ICUT(NC).EQ.0) GO TO 2179
NPNC = NP(NC)
DO 2178 K = 1, NPNC
ALPHA INC.K) = ALPHA(NC, K) - ZERON
2178 CONTINUE
2179 CONTINUE
C /* --------------- */
C /* FIT THE ABSORPTION COEFFICIENT TO A PARABOLA. */
C /* THIS SECTION IS SKIPPED IF IFIT = 1 */
C /* --------------- */
2180 CONTINUE
IF(IFIT.EQ.1) AA(1) = CPN
IF(IFIT.EQ.1) ZERON = 0.
C /* --------------- */
C /* OUTPUT THE ABSORPTION COEFFICIENT OF THE SAMPLE. */
C /* --------------- */
DO 179 NC = 1, NCUT
IF(ICUT(NC).EQ.0) GO TO 179
NPNC = NP(NC)
WRITE(6, 2) WRITE(6, 2)
WRITE(6, 10) RUN, (ADENT(K), K = 1, 15)
IF(IFIT.EQ.1) WRITE(6, 67) ZERON, CPN, CHISQR
IF(IFIT.EQ.1) WRITE(6, 45) AA(1), CHISQR
WRITE(6, 55)
DO 178 K = 1, NPNC
DO 178 K = 1, NPNC
WRITE(6, 46) K, V(NC, K), ALPHA(NC, K), RSALP(NC, K)
178 CONTINUE
179 CONTINUE
C /* --------------- */
C /* OUTPUT FITTED DATA ONTO UNIT 11. */
C /* --------------- */
C TZERO = ZERO + ZERON
WRITE(11, 2) ICUT(K), K = 1, NCUT, H, D, M, T, A
WRITE(11, 57) AA(1), AA(1), TZERO
DO 183 NC = 1, NCUT
IF(ICUT(NC).EQ.0) GO TO 183
WRITE (11, 10) BUN, (ADENT(F), K = 1, 15)
WRITE (11, 15) NP(NC), THICK(NC), NL(NC), WN(NC), WHP(NC), MATL(NC),
2 MAT(NC), WRITE (11, 19) ANASSA(NC), ANASSM(NC)
NPNC=NP(NC)
DO 107 K = 1, NPNC
WRITE (11, 20) K, V(NC, K), ALPHA(NC, K), RSALP(NC, K)
107 CONTINUE
183 CONTINUE
C
DEHORALIZE NORMALIZED ABSORPTION COEFFICENT IF INORM=1.
C
IF (INORM .NE. 1) GO TO 184
KX = NAL + 1
DO 1184 NC = 1, NCUT
IF (ICUT(NC) .EQ. 0) GO TO 1184
NPNC = NP(NC)
DO 1183 K = 1, NPNC
THCK = THICK(NC)
IF (KSS .LE. KK) CONST = ANASSA(NC) / (AREA * DALH * THICK(NC))
IF (KSS .LT. KK) CONST = ANASSM(NC) / (AREA * DALH * THICK(NC))
ALPHA(NC, K) = ALPHA(NC, K) * CONST
RSALP(NC, K) = RSALP(NC, K) * CONST
1183 CONTINUE
1184 CONTINUE
184 CONTINUE
C
PLOT ABSORPTION COEFFICENT ALONG WITH A LINE REPRESENTING
C THE FITTED POLYNOMIAL.
C
IF (ALPHA .NE. (0.0)) GO TO 187
ALPHA(NC) = 1
DO 186 NC = 1, NCUT
IF (ICUT(NC) .EQ. 0) GO TO 186
NL = NL(NC)
WHP(NC) = WHP(NC)
DO 185 K = NL, NCUT
V(K) = V(NC, K)
RRSDEV(K) = RSALP(NC, K)
185 CONTINUE
KX = NAL + 1
186 CONTINUE
EN = KX + 1
KX = NAL + 1
CALL SCALE(RRATIO, 10., MEN, AMIN, DELTA)
187 CONTINUE
THEO = 100. * AXIS
THEO = THEO
DEL = VMAX / THEO
WAVE = 0
DO 189 NC = 1, WSZTS
R = NC
IF (ICUT(NC) .NE. 0) GO TO 190
189 CONTINUE
190 CONTINUE
KK = NAL + 1
IF (KSS .GT. KK) CONST = ANASSM(K) / (AREA * DALH * THICK(K))
IF (KSS .LE. KK) CONST = ANASSA(K) / (AREA * DALH * THICK(K))
DO 195 K = 1, NCUT
WAVE = WAVE + DEL
VT(K) = WAVE
IF(INORM .GE. 1) TLT(K) = AA(1) * (WAV**2)
 IF(INORM .LT. 1) TLT(K) = CONST * AA(1) * (WAV**2)

195 CONTINUE
 CALL NUPLOT(TLT, AMIN, DELTAA, VT, VMIN, DELTAV, XAXIS, NTHEO,
 * ABSORPTION COEFFICIENT, 21, Wavenumber (cm-1)*, 16, 0, 0,
 * RUN, 1, ADENT, RUN, 0, ADENT)
 DO 210 NC=1, NCUT
   IF(ICUT(NC) .LE. 0) GO TO 210
   IF(VT(NC) .LE. 0) GO TO 210

   CALL BUPLOT(TLT, ABIN, DELTAAt,
   VTV, BIN, DELTAV, XAXIS, NTHEO,
   * ABSORPTION COEFFICIENT, 21, Wavenumber (cm-1)*, 16, 0, 0,
   * RUN, 1, ADENT, RUN, 0, ADENT)

   DO 209 K = 1, NEN
     ALPHA(NC, K) = ALPH(A(NC), K)
   DO 209 CONTINUE
   CALL LINE (TV, THIN, DELTAV, DBATIO, AMIN, DELTAA, NEN, -1, NC)

210 CONTINUE
 CALL PLOTE2

C*****************************************************************************
C STOKE VALUES FOR SUMMARY.
C*****************************************************************************

C
C SUMBUN(NSS) = RUN
C DO 250 K = 1, 15
C SUMADE(NSS, K) = ADENT(K)

250 CONTINUE
 COF(NSS) = AA(1)
 DCOF(NSS) = A(1)
 SUZERO(NSS) = ZEROW + ZERO

500 CONTINUE

C*****************************************************************************
C OUTPUT SUMMARY
C*****************************************************************************

C
KK = NSS - 1
 WRITE(6, 2)
 DO 525 L = 1, KK
   WRITE(6, 65) SUMBUN(L), COF(L), DCOF(L), SUZERO(L), (SUMADE(L, K), K = 1, 5)
525 CONTINUE

STOP
END
SUBROUTINE PAFIT(SI, SY, SSIGMA, NPTS, MODE, SA, DSA, SHISQR)

PURPOSE

MAKE A LEAST-SQUARES FIT TO DATA WITH A PARABOLA
ST = SA * (ST)**2

USAGE

CALL PAFIT(SI, SY, SSIGMA, NPTS, MODE, SA, DSA, SHISQR)

DESCRIPTION OF PARAMETERS

SI - ARRAY OF DATA POINTS FOR INDEPENDENT VARIABLE
SY - ARRAY OF DATA POINTS FOR DEPENDENT VARIABLE
SSIGMA - ARRAY OF STANDARD DEVIATIONS FOR Y DATA POINTS
NPTS - NUMBER OF PAIRS OF DATA POINTS
MODE - DETERMINES METHOD OF WEIGHTING LEAST-SQUARES FIT
+1 (INSTRUMENTAL) WEIGHT(I) = 1./SIGMA(I)**2
0 (NO WEIGHTING) WEIGHT(I) = 1.
-1 (STATISTICAL) WEIGHT(I) = Y(I)
SA - FREE PARAMETER
DSA - STANDARD DEVIATION OF FREE PARAMETER
SHISQR - REDUCED CHI SQUARE FOR FIT

SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED

NONE

DIMENSION STATEMENT VALID FOR NPTS UP TO 1000

REAL*8 SI(1), SY(1), SSIGMA(1)
REAL*8 WEIGHT, CHISQR, NUM, DEN, DA, DBLE

DO 25 K = 1, NPTS
    Y(K) = DBLE(SI(K))
    SY(K) = DBLE(SY(K))
    SIGHAY(K) = DBLE( SSIGMA(K) )

25 CONTINUE

CALCULATE A

NUM = 0.D0
DEN = 0.D0
DO 155 K = 1, NPTS
    IF (MODE.EQ.1) WEIGHT = 1.0D0/Y(K)
    IF (MODE.EQ.0) WEIGHT = 1.0D0
    IF (MODE.EQ.1) WEIGHT = SIGMA(K)
    TEST = SG1N(WEIGHT)
    IF (TEST .EQ. 0.0) WEIGHT = 1.0D0 - 0.7
    NUM = NUM + (I(K) / WEIGHT)**2 * I(K)
    DEN = DEN + (I(K)**2 / WEIGHT)**2
155 CONTINUE

A = NUM / DEN

CALCULATE THE STANDARD DEVIATION OF A

DA = 1.0D0 / DEN
DA = SQRT( DA )

CALCULATE CHISQR

CHISQR = 0.D0
DO 165 K = 1, NPTS
    IF (MODE.EQ.1) WEIGHT = 1.0D0/Y(K)
    IF (MODE.EQ.0) WEIGHT = 1.0D0
IF (MODE EQ 1) WEIGHT=SIGMAI(K)
TEST=SNGL(WIGHT)
IF (TEST EQ 0.0) WEIGHT=1.0D-07
CHISQR=CHISQR+((Y(K)-A*(X(K)**2))/WEIGHT)**2
165 CONTINUE
S)=SNGL(A)
DSE=SNGL(DA)
CHISQR=SNGL(CHISQR)
XNPTS=MPTS-1
MPDEF=XNPTS-1
CHISQR=CHISQR/MPFREE
RETURN
END
4) FIT

External References:

a) FCHISQR - A subroutine used to find the reduced value of $X^2$

b) GRIDLS - A subroutine intended to fit theoretical curves to experimental data.

Both of these subroutines are described fully by P.R. Bevington. 70,71
nnnnnnn

234

V A L U E S IS O U T P U T T E D O N T O U N I T 11.
dihe
EN
nS
: I O H V (5,520),
CK IS) , A D E N T (16)
7THICK
ENSlOfi
¥¥(3000) . B R A T I O (30001 ,RRS D E ¥ 13000) , A 120) ,AA(20) ,G (20)
dime
n:
EH SI O R UHI (20) ,fiD(20) . AWRI (20i .CD (20) ,A Vtf (20) ,ftCAP(20)
EH SI ON A L P H A (51520)
(5,520) , P
RSALP
(5000) ,’TT fF L { 55000)
000
DIHEHSI
S A L P (5,526)
(5,520) ,TLT(5000)
,fLT'(5000) ,¥T
;VT'(5000j
ENSIOH
HPI5)
,NL(5),Nh(5)
DIME
NSION H
P (5) ,tit(5)
,fih (5) ,NHP(5)
, NHPJ5)
DIB EH SI O N I C U T IS) -HATL (5) .MATH (5)
D I M E N S I O N SOMR UN (200) ,S U H A L E f 200,15) ,COF(200) ,D C O F J 2 00) , Z E R O (200)
D I M E NSION P A B B (20,20) , D P A R H (20,20) ,b 6 b DER (60) ,LORDER (60) ,
7S1GMA A (20)
COMMON/TPARS/HORDEB.IRHICH,ITHEO
2 F O R M A T (1H1)
4 FOBHAT (IX.5 1 1 , 1 2 , 2 F 6 . 2 , I X , 3 (G13.6 ,11) )
* FORMAT 1 b l 5 )5
7 F ORMAT
10 FORMAT
15 F ORMAT
19 F ORMAT
20 F ORMAT I 5 , 5 X , 3 ( E l S . 7 , 5 X I }
2 1 F O R M A T T S l S X . N (E15.7.5I)f
22 F OBHAT / / l l . ' & A W D A T * 1)
3 F O B H A T / / I X ,* DATA AFTER C O R R E C T I N G FOB D I M E N S I O N A L C H A R G E S 1)

25 FORMAT //IX,•CORRECTED ABSORPTION COEFFICENT1)
30 FOBHAT //IX,'NUMBER OF DATA POINTS•,22X,I5/1X,
? •THICKNESS OF SAMPLE1,
724I.E15.7/1X,'INLEX OF LOWEST USEABLE POINT',1«I,I5/1X,
F'IN&EI OF HIGHEST USEABLE POINT (FOR FIT) •,31,15/11,
7 •INDEXOF H1GEST USEABLE POINT (FOB PLOT)*,3X,15)
32 FORMAT(IX,•INDEX OF POINT US EL TO HATCH CUTOFFAT LOWER END1,7X,
715/1X,•INDEX OF POINT USED TO HATCH CUTOFF AT UPPER END',7X,I5)
33 FOBHAT(IX,'TYPE OF ALUM IN A= ',12/IX,
7 •AREA OF 5A HPLE = • G15.7.' CH**2'/1X,
7*DENSITX OF ALUMINA* '.Gl5.7,' GHAHS PER CC.'/IX,
7 •DENSITI OF METAL- ',Gl5.7,1 GRAMS PEB CC.'/1X,
?'ZERO= *,G15.7)
34 FOHHAT(1X,'HYDROGEN CONTENT= ',12
7/11,•HASS OF ALUM1NA* '.G15.7
H A ¥ E NUMBER (CM -1)

41,'ABSORPTION CDEFF-*

6 0 F ORMAT / / Ill 'SAMPLE *, 5 X ”, 'COF • , 171. ' D C O F 1 , 13X , »ZEHO' , 13X , 'LABEL*)
6 5 F OBHAT i X , F 6 . 2 , 3 ( 5 l , E l 5 . 7 ) , 2 X , 6 A 4 f
, 3 (E1 5 . 7 , 5 f ) )
67 F ORMAT 1 1 .3(1
70 F O R M A T I X . 3012)
71 F O R M A T / / I X , ' B O R D E R * ', IX , 301 2)
M E T E R S FOR D I H E N S I O N A L C H A N G E S •//
7 2 F O R H A T L/ / I X , ' P A R A_______
761,'FRACTloSlL
CONTRACTION
A C T I O N A L LINEAR
L I N E A R THERMAL
THERMAL C
O N T R A C T I O N OF SAMPLE
S A M P L E BOLDER*

7E15.7//

7
6A
1•
, 'fFDHL
RACT
A L LI NEAR
IU
1I
AVO N
Pdw
■£< HD T H E R M A L E X P A N S I O N OF P A L L A D Z U H D P O N
7 ' H T D R I D I H G * ' ,1X,£15.7)
73 F O P M A T I 1 X , « (G13-6 . 2 X ) )
AATTfI////i1XX,_
IN E F F E C T : './ I X , •1 F I T * ',3 X ,1 5 / 1 X , *I C O R * •,,3X,
7 4 715/
F OB
R MM
» 'OPTIONS I
______
/ I X , fl P L O T-= '-, 2-X . 1 5 / 1 X , ' I W H ICH*' , 1X ,-I 5/II, * 1 T H E O * • , 2 l , 1 5)
75 FOrrfSA T ( I X , ' C O F * * , 5 l , E l 5 . 7 / 1 1 , 'DCOP* * , 1 X , E 15.7/11,
7 * F C I = ' , 2 X , E 13.6)
^
7 1 X , ' S T A N D A R D D E V I A T I O N O F LN OF P A R T I C L E D I A M E T E R S * 1 , 2 X ,E 1 5 . 7 /
7 1 1 , ' D I A H E T E H O F P A R T I C L E S * • , 2 1 (E 1 5 . 7 /
F I X , ' S T A N D A R D D E V I A T I O N O F LN OF C L U S T E R D I A H E T E F S * • , 2 1 , E 1 5 . 7 /
7 1 X , ' P L A S M A F R E Q U E N C S * ' , 2 1 , E 1 5.7/
7 1 X , ' F E R M I V E L O C I T Y * • , 2 X , E i 5 . 7/


FILLING FRACTION OF METAL INSIDE CLUSTERS, 2X, E15.7/
RELAXATION TIME (SEC), 2X, E15.7/
COF, 2X, E15.7/
ZERO, 2X, E15.7/
AREA, 2X, E15.7/
THICKNESS, 2X, E15.7/
FRACTIONAL LINEAR THERMAL CONTRACTION OF METAL, 2X, E15.7/
DENSIY OF ALUMINA, 2X, E15.7/
STANDARD DEVIATION OF LN OF PARTICLE DIAMETERS, 2X, E15.7/
AVARAGE OF LN OF PARTICLE DIAMETERS, 2X, E15.7/
STANDARD DEVIATION OF LN OF CLUSTER DIAMETERS, 2X, E15.7/
VOLUME WEIGHTED PARTICLE DIAMETER SIZE DISTRIBUTION, 2X, E15.7/
VOLUME WEIGHTED PARTICLE DIAMETER (CM), 2X, E15.7/
VOLUME WEIGHTED RECIPROCAL OF DIAMETER, 2X, E15.7/
MEAN PARTICLE DIAMETER (CM), 2X, E15.7/
VOLUME WEIGHTED CLUSTER DIAMETER SIZE DISTRIBUTION, 2X, E15.7/
VOLUME WEIGHTED CLUSTER DIAMETER (CM), 2X, E15.7/
MEAN CLUSTER DIAMETER (CM), 2X, E15.7/
ALUMINA FILLING FRACTION, 2X, E15.7/
DIELECTRIC FUNCTION OF HOST (ASSUMED REAL), 2X, E15.7/
INITIAL REDUCED CHISQ, 2X, E15.7/
REDUCED CHISQ ON PASS, 2X, E15.7/
STANDARD DEVIATION OF FITTED VALUE, 2X, E15.7/
STANDARD DEVIATION OF FITTED VALUES, 2X, E15.7/
STANDARD DEVIATION OF FITTED PARAMETERS, 2X, E15.7/
STANDARD DEVIATION OF ORIGINAL DATA, 2X, E15.7/
STANDARD DEVIATION OF SAMPLE, 2X, E15.7/
STANDARD DEVIATION OF ACTION, 2X, E15.7/
PLASMA FREQUENCY, 2X, E15.7/
AVE OF LN OF PART DIAM, 2X, E15.7/
ST. DEV OF LN OF PART DIAM, 2X, E15.7/
OVERALL FILL FRACTION, 2X, E15.7/
CLUSTER FILL FRACTION, 2X, E15.7/
AVE OF LN OF CLUS DIAM, 2X, E15.7/
ST. DEV OF LN OF CLUS DIAM, 2X, E15.7/
MEAN FREE PATH (MICRONS), 2X, E15.7/
FERMI VELOCITY (CM/SEC), 2X, E15.7/
LAMBO OFFSET (CM-1), 2X, E15.7/
RELAXATION TIME (SFC), 2X, E15.7/
HOST DIE FUNCTION, 2X, E15.7/
CLUSTER DIAMETER, 2X, E15.7/
PARTICLE DIAMETER, 2X, E15.7/

DATA G (1), 2.93134062E-4/
DATA G (2), 2.279703625E-3/
DATA G (3), 4.05975362E-2/
DATA G (4), 2.417303375E-1/
DATA G (5), 2.34292492548026E-1/
DATA G (6), 2.417303375E-1/
DATA G (7), 2.59736362E-2/
DATA G (8), 2.79703625E-3/
DATA G (9), 2.252314062E-4/
DATA G (10), 1.37663562E-2/
DATA G (11), 3.944404256E-3/
DATA G (12), 4.01286E-11/
DATA MC01/7/
DATA MC01/7/
DATA MC01/7/
DATA G (14), 1867902/
DATA MC01/7/
CALL PLOT(0.,0.,1)
WRITE(6,2)

READ A CARD TO DETERMINE PROGRAM MODE.

IFIT = 0 SKIP FITTING SECTION
      = 1 FIT DATA TO THEORY

ICON = 0 CORRECT DATA FOR DIMENSIONAL CHANGES
      = 1 DO NOT CORRECT DATA FOR DIMENSIONAL CHANGES

IPLAN = 0 PLOT DATA ONLY
       = 1 PLOT DATA AND PARABOLIC LINE
       = 2 PLOT DATA, PARABOLIC LINE, AND THEORETICAL CURVE

IWHICH = 0 MEAN FREE PATH IS TAKEN TO BE THE RADIUS OF THE
        PARTICLE (MICRONS)
       = 1 MEAN FREE PATH IS TAKEN TO BE GIVEN BY A LOG
          NORMAL DISTRIBUTION
       = 2 RELAXATION TIME IS FIT DIRECTLY TO BULK DIELECTRIC
          FUNCTION INSTEAD OF BEING CALCULATED FROM THE FERMI
          VELOCITY AND THE MEAN FREE PATH.

ITHEO = 1 FIT DATA USING CMIEL
       = 2 FIT DATA USING ECHIEL
       = 3 FIT DATA USING CMIEP
       = 4 FIT DATA USING ECHIEP
       = 5 FIT DATA USING CLUS
       = 6 FIT DATA USING ECLUS
       = 7 FIT DATA USING IMIEL
       = 8 FIT DATA USING EIMI
       = 9 FIT DATA USING EDDY
      =10 FIT DATA USING EDDY

THE READ FORMAT IS (515).

READ(5,5) IFIT, ICON, IPLAN, IWHICH, ITHEO
WRITE(6,71) IFIT, ICON, IPLAN, IWHICH, ITHEO
WRITE(11,5) IFIT, ICON, IPLAN, IWHICH, ITHEO

READ A CARD TO DETERMINE WHICH PARAMETERS ARE TO BE FIT AND
WHICH ORDER THEY ARE TO BE FITTED.

READ LORDER

DISCRION OF PARAMETERS:
PARK(1) = PLASMA FREQUENCY OF METAL (EV)
PARK(2) = AVERAGE OF LN OF PARTICLE DIAMETERS (LN(MICRONS))
PARK(3) = STANDARD DEVIATION OF LN OF PARTICLE DIAMETERS
PARK(4) = OVERALL FILLING FRACTION
PARK(5) = CLUSTER FILLING FRACTION
PARK(6) = AVERAGE OF LN OF CLUSTER DIAMETERS (LN(MICRONS))
PARK(7) = STANDARD DEVIATION OF LN OF LN OF CLUSTER DIAMETERS
PARK(8) = MEAN FREE PATH OF BULK MATERIAL (CM/S)
PARK(9) = FERMI VELOCITY OF METAL (CM/SEC)
PARK(10) = ZERO OFFSET
PARK(11) = RELAXATION TIME (SEC)
PARK(12) = DIELECTRIC FUNCTION OF HOST (ASSUMED REAL)
PARK(13) = CLUSTER DIAMETER
PARK(14) = PARTICLE DIAMETER

THE READ FORMAT IS (IX,10I2)

READ(5,70) (LORDER(K), K=1,NUMPARK)
WRITE(6,71) (LORDER(K), K=1,NUMPARK)
WRITE(11,70) (LORDER(K), K=1,NUMPARK)
WRITE(6,70) (PARK(K), K=1,NUMPARK)
WRITE(11,70) (PARK(K), K=1,NUMPARK)
COUNT NUMBER OF PARAMETERS TO BE FITTED.

NPARM=0
DO 1110 K=1,NUPMIPC
   IF(LORDER(K).EQ.0) GO TO 1111
   NPARM=K
1110 CONTINUE
1111 CONTINUE

COPY LORDER INTO BORDER.

DO 1112 K=1,NPARM
   ORDER(K)=ORDER(K)
1112 CONTINUE

LL=NUPMICH
DO 1120 K=1,NUPMICH
   IF(NORDER(K).NE.QORDER(L)) GO TO 1120
   QORDER(L)=QORDER(K)
1120 CONTINUE
IF(NPARM.EQ.0)IPIT=0

READ A CARD WITH PLOTTING PARAMETERS.

READ(5,50)XMAX,XAXIS,XALPHA
WRITE(11,50)XMAX,XAXIS,XALPHA
DELTAB=XMAX/XAXIS
VMAX=0.

READ A CARD WITH PARAMETERS FOR DIMENSIONAL CHANGES

THRESH=FRACTIONAL LINEAR THERMAL CONTRACTION OF SAMPLE HOLDER
HYDEXP=FRACTIONAL LINEAR THERMAL EXPANSION OF PALLADIUM UPON
THE READ FORMAT IS (F6.0,5X,3(F7.5,X)).

READ(5,7) DUM, THEMS, HYDEXP
WRITE(6,72) THEMS, HYDEXP
DUM=0.
WRITE(11,7) DUM, THEMS, HYDEXP

READ THE FOLLOWING PARAMETERS:
AREA = THE AREA OF THE SAMPLE HOLDER IN CM**2
THE READ FORMAT IS (F6.4).

READ(5,7) AREA

CORRECT AREA OF SAMPLE HOLDER FOR THERMAL CONTRACTION.
IF (ICOR.EQ.0.) AREA=AREA*((1.-THEMS)**2)
WRITE(11,7) AREA
DO 500 NNS=1, NSETS
ALPHA=ALPHA

READ WHICH CUTOFFS ARE PRESENT
ICUT(1)>1 = 26 CM-1 CUTOFF IS PRESENT
ICUT(2)>1 = 60 CM-1 CUTOFF IS NOT PRESENT
ICUT(3)>1 = 110 CM-1 CUTOFF IS NOT PRESENT
ICUT(4)>1 = 200 CM-1 CUTOFF IS NOT PRESENT
ICUT(5)>1 = 300 CM-1 CUTOFF IS NOT PRESENT
ICUT(6)>1 = 400 CM-1 CUTOFF IS NOT PRESENT

NOTE: IF ICUT FOR ANY CUTOFF IS EQUAL TO 1, THAT CUTOFF IS
SKIPPED WHEN THE FITTING IS DONE.

DETERMINE WHICH TYPE OF ALUMINA IS PRESENT
HALU = 3 LlNDE B
= 2 LlNDE C
= 3 LlNDE 0.3 MICRON
< 1 TERMINATE EXECUTION

READ SAMPLE CHARACTERISTICS:
DALUM = THE DENSITY OF THE ALUMINA IN THE SAMPLE
DMEtal = THE DENSITY OF THE METAL IN THE SAMPLE
ALPHA = HIGHEST VALUE OF ALPHA/F.
THEMS = THEORETICAL LINEAR THERMAL CONTRACTION OF METAL
THERMA = FRACTIONAL LINEAR THERMAL CONTRACTION OF ALUMINA
THE READ FORMAT IS (1X,5F11.6,4F22.6,12,3(F13.6,12)).

(IF NAL<1, BRANCH TO SUMMARY SECTION.)

READ(5,8) ICUT(K), K=1, NCUT, HALU, DALUM, DMEtal, ALPHA, THERM, THERMA
IF (ALPHA.LT.4.0) ALPHA=ALPHA
DELTA=ALPHA/10.
AMINO=0.
IF (HALU.LT.1.) GO TO 501

READ IN SIMPLE CHARACTERISTICS.

COP = COEFFICIENT OF LEAST-SQUARE FIT TO A PARABOLA
DSOP = STANDARD DEVIATION OF COP
The value to be subtracted from the normalized absorption is:

```
READ (5, 67) COP (NSS), DCOP (NSS), ZERO (NSS)
```

**Read in sample characteristics (continued).**

- **RLA** = Average of LN of particle diameters LN(MICRONS)
- **RLS** = Standard deviation of LN of particle diameters LN(MICRONS)
- **CLA** = Average of LN of cluster diameters LN(MICRONS)
- **CLS** = Standard deviation of LN of cluster diameters LN(MICRONS)

```
READ (5, 73) RLA, RLS, CLA, CLS
```

**Read in sample characteristics (continued).**

- **XPATH** = Mean free path of bulk material (MICRONS)
- **WP** = Plasma frequency of metal (EV)
- **FERM** = Fermi velocity of metal (CM/SEC)
- **PCI** = Filling fraction of metal in clusters

```
READ (5, 73) XPATH, WP, FERM, PCI
```

**Read in sample characteristics (continued).**

- **RTIME** = Relaxation time in sec.

```
READ (5, 73) RTIME
```

**Bead in the first header card.**

This card is for identification only. It consists of a 5 digit real number and a 60 space title. Each cutoff must have a first header card, but only the first header card of the last cutoff is used.

```
DO 105 HC=1,NCUT IF (ICUT (NC) .EQ.0) GO TO 105
```

**Bead in the second header card.**

- **NP (NC)** = Number of data points
- **THICK (NC)** = Thickness of the sample in CM.
- **ML (NC)** = Index of the lowest useable data point
- **MH (NC)** = Index of the highest useable data point (for plot)
- **HWP (NC)** = Index of the highest useable data point (for plot)
- **MATL (NC)** = Index corresponding to point equivalent to point designated in next lower cutoff.
- **MATH (NC)** = Index corresponding to point equivalent to point designated in next lower cutoff.

```
READ (5, 10) RUN, (ADENT (K), K=1, 15)
```

**Bead in the third header card.**

- **NP (NC)** = Number of data points
- **THICK (NC)** = Thickness of the sample in CM.
- **ML (NC)** = Index of the lowest useable data point
- **MH (NC)** = Index of the highest useable data point (for plot)
- **HWP (NC)** = Index of the highest useable data point (for plot)
- **MATL (NC)** = Index corresponding to point equivalent to point designated in next lower cutoff.
- **MATH (NC)** = Index corresponding to point equivalent to point designated in next lower cutoff.

```
READ (5, 15) NP (NC), THICK (NC), ML (NC), MH (NC), HWP (NC), MATL (NC), MATH (NC)
```

**Read in the third header card.**
DETERMINE HYDROGEN CONTENT

\[ IHY = 0 \Rightarrow \text{SAMPLE WAS NOT SOAKED IN HYDROGEN} \]
\[ = 1 \Rightarrow \text{SAMPLE WAS SOAKED IN HYDROGEN} \]

DETERMINE SAMPLE MASSES

\[ M_{\text{SAM}} = \text{MASS OF THE ALUMINA IN THE SAMPLE (GRAMS)} \]
\[ M_{\text{MET}} = \text{MASS OF THE METAL IN THE SAMPLE (GRAMS)} \]

THE READ FORMAT IS \( (15,5,3,(E15.7,5)) \)

READ \((5,19) \) IHY, MASSA(NC), MASSM(NC)

READ IN POINTS AND THEIR STANDARD DEVIATIONS.

\[ K = \text{INDEX} \]
\[ \text{WAVENUMBER (CM}^{-1}) \text{) } \]
\[ \text{ALPHA(K) = NORMALIZED ABSORPTION COEFFICIENT} \]
\[ \text{BSALP(K) = STANDARD DEVIATION OF THE NORMALIZED ABSORPTION} \]

THE READ FORMAT IS \( (15,5,3,(E15.7,5)) \)

\[
\text{NPNC} = \text{NP}(\text{NC})
\]
\[
\text{DO 101 K=1,NPNC}
\]
\[
\text{READ} (5,20) IPX, V(\text{NC},K), \text{ALPHA(\text{NC},K)}, \text{BSALP(\text{NC},K)}
\]
\[
101 \text{ CONTINUE}
\]
\[
105 \text{ CONTINUE}
\]

OUTPUT RAW DATA

\[
\text{DO 109 NC=1,NCUT}
\]
\[
\text{IF} (\text{ICUT(\text{NC}) .EQ.0}) \text{GO TO 109}
\]
\[
\text{WRITE} (6,2)
\]
\[
\text{WRITE} (6,22)
\]
\[
\text{WRITE} (6,30) NP(\text{NC}), \text{THICK(\text{NC})}, \text{WL(\text{NC})}, \text{WH(\text{NC})}, \text{WP(\text{NC})}
\]
\[
\text{WRITE} (6,32) \text{MA2L(\text{NC})}, \text{MA3TH(\text{NC})}
\]
\[
\text{WRITE} (6,34) \text{AMASSA(\text{NC})}, \text{AMASSM(\text{NC})}
\]
\[
\text{WRITE} (6,75) \text{CUP(\text{NSS}), DCOP(\text{NSS}), PCIRLA, RLS, IPATH, CLA, CLS, WP, PERM, PCI, RTIME}
\]
\[
\text{WRITE} (6,53) \text{ALU, AREA, DLM, DMETAL, ZER0(\text{NSS})}
\]
\[
\text{WRITE} (6,55)
\]
\[
\text{NPNC} = \text{NP}(\text{NC})
\]
\[
\text{DO 107 K=1,NPNC}
\]
\[
\text{WRITE} (6,20) \text{K}, V(\text{NC},K), \text{ALPHA(\text{NC},K)}, \text{RSALP(\text{NC},K)}
\]
\[
107 \text{ CONTINUE}
\]
\[
109 \text{ CONTINUE}
\]
\[
\text{IF} (\text{ICOF .NE.0}) \text{GO TO 170}
\]

CORRECT DATA FOR THERMAL CONTRACTION OF METAL AND ALUMINA.

\[
\text{DO 117 NC=1,NCUT}
\]
\[
\text{CONST} = 1. / ((1. - \text{THEMMA}) ** 3)
\]
\[
\text{IF} (\text{ICUT(\text{NC}) .EQ.0}) \text{GO TO 117}
\]
\[
\text{MPC} = \text{MP}(\text{NC})
\]
\[
\text{DO 115 K=1,NPNC}
\]
\[
\text{ALPHA(\text{NC},K)} = \text{CONST} \times \text{ALPHA(\text{NC},K)}
\]
\[
\text{RSALP(\text{NC},K)} = \text{CONST} \times \text{BSALP(\text{NC},K)}
\]
\[
115 \text{ CONTINUE}
\]
\[
\text{COP(\text{NSS}) = COP(\text{NSS}) \times \text{CONST}}
\]
\[
\text{DCOP(\text{NSS}) = DCOP(\text{NSS}) \times \text{CONST}}
\]
\[
\text{ZERO(\text{NSS}) = ZERO(\text{NSS}) \times \text{CONST}}
\]
\[
\text{DMETAL = DMETAL \times \text{CONST}}
\]
\[
\text{DALUM = DALUM / ((1. - \text{THEMMA}) ** 3)}
\]
BLA=BLA+ALOG(1.-THEM)
CLA=CLA+ALOG(1.-THEM)
IF(INV.NE.1) GO TO 129

**CORRECT DATA FOR THE EXPANSION OF THE METAL WITH HYDROGEN**

ABSOP: (IEO) 

IF (IHT.NE.1) GO TO 129
CORRECT DATA FOR THE EXPANSION OF THE PETAL WITH HT DROSET AB50RTIOK.

(THE ONLY EFFECTS THOSE SAMPLES WITH HYDROGEN)

THIS SECTION IS SKIPPED IF ICOF=1.

**CORRECT DATA FOR THE EFFECTS OF THE THERMAL CONTRACTION OF THE SAMPLE HOLDER.**

THIS SECTION IS SKIPPED IF ICOF=1.

**OUTPUT DATA AFTER CORRECTING FOR DIMENSIONAL CHANGES.**

THIS SECTION IS SKIPPED IF ICOF=1.

**END OF PROGRAM**

WRITE (6, 1) IC, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICUT, ICU
DETERMINE THE VOLUME WEIGHTED PARTICLE DIAMETER.

AMLDIA = \exp \left( \frac{1}{E4} \right)
AVR = 0.
BCA = 0.
ACC = 0.
DAR = RLA - 4 * RLS
DO 170 K = 1, 12
BD(K) = \exp \left( \frac{DAR}{E4} \right)
BC = RD(K) * 3
WHI(K) = G(K) * RC
ACC = ACC + WHI(K)
DAR = DAR + RLS
AVR(K) = BV(K) * WHI(K)
AVR = AVR + AVR(K)
RCAP(K) = WHI(K) / RD(K)
BCA = RCA + RCAP(K)
170 CONTINUE
AVR = AVR / ACC
BCA = RCA / ACC
WRITE (6, 80)
DO 171 K = 1, 12
AVR(K) = AVR(K) / ACC
WHI(K) = WHI(K) / ACC
AVC = AVC + AVR(K)
171 CONTINUE
AVC = AVC / ACC
WRITE (6, 81) AVR, RCA, AMEDIA

DETERMINE THE VOLUME WEIGHTED CLUSTER DIAMETER.

ACDIA = \exp \left( \frac{CLA}{E4} \right)
AVC = 0.
ACC = 0.
DAR = CLA - 4 * CLS
DO 173 K = 1, 12
CD(K) = \exp \left( \frac{DAR}{E4} \right)
BC = CD(K) * 3
WHI(K) = G(K) * RC
ACC = ACC + WHI(K)
DAR = DAR + CLS
AVC(K) = CD(K) * WHI(K)
AVC = AVC + AVC(K)
173 CONTINUE
AVC = AVC / ACC
WRITE (6, 84)
DO 174 K = 1, 12
AVC(K) = AVC(K) / ACC
WHI(K) = WHI(K) / AVC(K)
174 CONTINUE
WRITE (6, 85) AVC, CMEDIA

CALCULATE METAL AND ALUMINA FILLING FRACTIONS.

K = NC
IF (ICUT(WC) .NE. 0) GO TO 172
171 CONTINUE
FILLA = MASSA(K) / (DALUM * AREA * THICK(K))
FILLI = MASSI(K) / (DMETAL * AREA * THICK(K))

FIND DIELECTRIC CONSTANT OF HOST (ASSUMED REAL).

CALL EPOLE(EP1, EP2, 9.61, 0., 0., 0., XL, XL, XL)
CALL MAIGAR (RF1,RF2,PP1,PE2,1.,0.,FILLA)
WRITE (6,67) FILLA,FILLA,NE1
C*****************************************************************************
C LOAD FITTING PARAMETER ARRAY ACCORDING TO ORDER.
C*****************************************************************************
PAM (NSS,1) = WP
PAM (NSS,2) = RLA
PAM (NSS,3) = RLS
PAM (NSS,4) = PILLM
PAM (NSS,5) = FCI
PAM (NSS,6) = CLA
PAM (NSS,7) = CLS
PAM (NSS,8) = XPATR
PAM (NSS,9) = PERM
PAM (NSS,10) = RTIME
PAM (NSS,11) = RC1
PAM (NSS,12) = RC1
PAM (NSS,13) = RC1
PAM (NSS,14) = RC1
DO 173 K = 1, NUMPAR
   DPAM (NSS,K) = 0.1*PAM (NSS,K)
173 CONTINUE
DO 174 K = 1, NUMPAR
   L = ORDER (K)
   A (F) = PAM (NSS,L)
   AA (K) = DPAM (NSS,L)
IF (AA (K) .EQ. (0.0)) AA (K) = 0.1
174 CONTINUE
IF (IFIT .EQ. 0) GO TO 180
C*****************************************************************************
C LOAD ABSORPTION COEFFICIENT INTO FITTING ARRAYS.
C (THIS SECTION IS SKIPPED IF IFIT=0)
C*****************************************************************************
NST-1 DO 176 RC*
   IF (ICUT (NC) .LE. 1) GO TO 176
   KST=NH (NC)-NL (NC)+1
   NW=KST+XST-1
   NLNC=NL (NC)
   WHRC=NH (NC)
   KK=NST-1
   DO 175 K=NLNC,WHRC
      VV (KK)=V (NC, K)
      RRAT (KK)=ALPHA (NC, K)
      RRSDEV (KK)=RSALP (NC, K)
175 CONTINUE
NST=NST+1
176 CONTINUE
C*****************************************************************************
C FIT THE ABSORPTION COEFFICIENT TO THEORY.
C (THIS SECTION IS SKIPPED IF IFIT=0)
C*****************************************************************************
WRITE (6, 21) NUMPR=NUMPR
IF (NUMPR .GT. 4) NUMPR=4
DO 1175 K=1,NEN
   TFL (K) = FUNCTN (VV, K, A)
1175 CONTINUE
NUMFE=NUMPR
CALL GRIDIS (RM, NRATIO, RRSDEV, NEN, MP3EE, 1, TFL)
WRITE (6, 91) CHISOR, (A (KKL), KKL=1, NUMPR)
DO 1177 K=1, 7
   CALL GRIDIS (VV, RM, NRATIO, RRSDEV, NEN, MP3EE, 1, A, AA, SIGMA, TFL, CHISOR)
   WRITE (6, 93) K, CHISOR, (A (KKL), KKL=1, NUMPR)
1177 CONTINUE
C UNLOAD FITTING PARAMETER ARRAY ACCORDING TO NORDER.
C (THIS SECTION IS SKIPPED IF IFIT=0)
C
DO 1176 K=1,NUMPAR
  L=NORDER(K)
  PARM(NSS,L)=A(K)
  DPARM(NSS,L)=SIGMAA(K)
1176 CONTINUE
  WP=PARM(NSS,1)
  FLA=PARM(NSS,2)
  BLS=PARM(NSS,3)
  PTLL=PARM(NSS,4)
  FCI=PARM(NSS,5)
  CLS=PARM(NSS,6)
  CLR=PARM(NSS,7)
  XPATH=PARM(NSS,8)
  FERM=PARM(NSS,9)
  ZERO(NSS)=PARM(NSS,10)
  RT=E=PARM(NSS,11)
  HET=PARM(NSS,12)
  AVC=PARM(NSS,13)
  AYF=PARM(NSS,14)
C
C OUTPUT FITTED PARAMETERS.
C (THIS SECTION IS SKIPPED IF IFIT=0)
C
WRITE (6,2)
WRITE (6,830)
WRITE (6,835)
DO 179 K=1,NUMPAR
  N=NORDER(K)
  GO TO (801,802,803,804,805,806,807,808,809,810,811,812,813,814),N
  801 WRITE (6,901) N
  GO TO 178
  802 WRITE (6,902)
  GO TO 178
  803 WRITE (6,903)
  GO TO 178
  804 WRITE (6,904)
  GO TO 178
  805 WRITE (6,905)
  GO TO 178
  806 WRITE (6,906)
  GO TO 178
  807 WRITE (6,907)
  GO TO 178
  808 WRITE (6,908)
  GO TO 178
  809 WRITE (6,909)
  GO TO 178
  810 WRITE (6,910)
  GO TO 178
  811 WRITE (6,911)
  GO TO 178
  812 WRITE (6,912)
  GO TO 178
  813 WRITE (6,913)
  GO TO 178
  814 WRITE (6,914)
  178 CONTINUE
WRITE (6,840) PARM(NSS,N), DPARM(NSS,N)
179 CONTINUE
180 CONTINUE
C
C OUTPUT FITTED DATA ONTO UNIT 11.
C DRAW RACKING FOR CHARACTERISTIC CURVE AND THERMAL CURVE ALONG WITH
C DRAW REAL RACKING IN ISOTREDIP PVC PLOTS (TAFPA=0) OR
C PLOD REAL RACKING FOR PLOTTING PLOTS
C
C 107 CONTINUE
C
C 108 CONTINUE
C
C 109 CONTINUE
C
C 110 CONTINUE
C
C 111 CONTINUE
C
C 112 CONTINUE
C
C 113 CONTINUE
C
C 114 CONTINUE
C
C 115 CONTINUE
C
C 116 CONTINUE
C
C 117 CONTINUE
C
C 118 CONTINUE
C
C 119 CONTINUE
C
C 120 CONTINUE
C
C 121 CONTINUE
C
C 122 CONTINUE
C
C 123 CONTINUE
C
C 124 CONTINUE
C
C 125 CONTINUE
C
C 126 CONTINUE
C
C 127 CONTINUE
C
C 128 CONTINUE
C
C 129 CONTINUE
C
C 130 CONTINUE
C
C 131 CONTINUE
C
C 132 CONTINUE
C
C 133 CONTINUE
C
C 134 CONTINUE
C
C 135 CONTINUE
C
C 136 CONTINUE
C
C 137 CONTINUE
C
C 138 CONTINUE
C
C 139 CONTINUE
C
C 140 CONTINUE
C
C 141 CONTINUE
C
C 142 CONTINUE
C
C 143 CONTINUE
C
C 144 CONTINUE
C
C 145 CONTINUE
C
C 146 CONTINUE
C
C 147 CONTINUE
C
C 148 CONTINUE
C
C 149 CONTINUE
C
C 150 CONTINUE
C
C 151 CONTINUE
C
C 152 CONTINUE
C
C 153 CONTINUE
C
C 154 CONTINUE
C
C 155 CONTINUE
C
C 156 CONTINUE
C
C 157 CONTINUE
C
C 158 CONTINUE
C
C 159 CONTINUE
C
C 160 CONTINUE
C
C 161 CONTINUE
C
C 162 CONTINUE
C
C 163 CONTINUE
C
C 164 CONTINUE
C
C 165 CONTINUE
C
C 166 CONTINUE
C
C 167 CONTINUE
C
C 168 CONTINUE
C
C 169 CONTINUE
C
C 170 CONTINUE
C
C 171 CONTINUE
C
C 172 CONTINUE
C
C 173 CONTINUE
C
C 174 CONTINUE
C
C 175 CONTINUE
C
C 176 CONTINUE
C
C 177 CONTINUE
C
C 178 CONTINUE
C
C 179 CONTINUE
C
C 180 CONTINUE
C
C 181 CONTINUE
C
C 182 CONTINUE
C
C 183 CONTINUE
C
C 184 CONTINUE
C
C 185 CONTINUE
C
C 186 CONTINUE
C
C 187 CONTINUE
C
C 188 CONTINUE
C
C 189 CONTINUE
C
C 190 CONTINUE
C
C 191 CONTINUE
C
C 192 CONTINUE
C
C 193 CONTINUE
C
C 194 CONTINUE
C
C 195 CONTINUE
C
C 196 CONTINUE
C
C 197 CONTINUE
C
C 198 CONTINUE
C
C 199 CONTINUE
C
C 200 CONTINUE
C
C 201 CONTINUE
C
C 202 CONTINUE
C
C 203 CONTINUE
C
C 204 CONTINUE
C
C 205 CONTINUE
C
C 206 CONTINUE
C
C 207 CONTINUE
C
C 208 CONTINUE
C
C 209 CONTINUE
C
C 210 CONTINUE
C
C 211 CONTINUE
C
C 212 CONTINUE
C
C 213 CONTINUE
C
C 214 CONTINUE
C
C 215 CONTINUE
C
C 216 CONTINUE
C
C 217 CONTINUE
C
C 218 CONTINUE
C
C 219 CONTINUE
C
C 220 CONTINUE
C
C 221 CONTINUE
C
C 222 CONTINUE
C
C 223 CONTINUE
C
C 224 CONTINUE
C
C 225 CONTINUE
C
C 226 CONTINUE
C
C 227 CONTINUE
C
C 228 CONTINUE
C
C 229 CONTINUE
C
C 230 CONTINUE
C
C 231 CONTINUE
C
C 232 CONTINUE
C
C 233 CONTINUE
C
C 234 CONTINUE
C
C 235 CONTINUE
C
C 236 CONTINUE
C
C 237 CONTINUE
C
C 238 CONTINUE
C
C 239 CONTINUE
C
C 240 CONTINUE
C
C 241 CONTINUE
C
C 242 CONTINUE
C
C 243 CONTINUE
C
C 244 CONTINUE
C
C 245 CONTINUE
C

45
C

KK=1
DO 190 NC=1,NCUT
IF (ICUT(NC).NE.0) KK=NC
190 CONTINUE
JH=NH(KK)
PRAX=V(KK)
THEO=10.*KAXIS
NTHPO=THEO
DFL=VAX/THEO
WAV0.
DO 195 K=1,NTHEO
WAV=WAV+DEL
VT(K)=WAV
IF (VT(K)-CT.PRAX) GO TO 197
IF (IPLT.EQ.0.OR.IPLT.EQ.3) TLT(K)=COF(NSS)+(WAV**2)
IF (IPLT.EQ.0.OR.IPLT.EQ.2) TLT(K)=0.
IF (IPLT.EQ.2.OR.IPLT.EQ.3) TFL(K)=FUNCTN(VT,K,A)
195 CONTINUE
NTHPO=KK-1
CALL SC3TPT (LT,AMIN,DELTA,VT,WIN,DELTAV,TAXIS,WTHEO,
?ABSORPTION COEFFICIENT, 21, WAVENUMBER (CM-1), 16, 0, 0,
?FUN, 1, ADENT, RUN, 0, ADPNT)
DO 210 NC=1,NCUT
IF (ICUT(NC).EQ.0) GO TO 210
NLNC=NL(NC)
NHPNC=NHP(NC)
NEW=NHPNC-NEW+1
DO 209 K=1,NEW
KK=KK+1
K1=K
K2=2
197 CONTINUE
NTHPO=KK-1
CALL SC3TPT (LT,AMIN,DELTA,VT,WIN,DELTAV,TAXIS,WTHEO,
?ABSORPTION COEFFICIENT, 21, WAVENUMBER (CM-1), 16, 0, 0,
?FUN, 1, ADENT, RUN, 0, ADPNT)
DO 210 NC=1,NCUT
IF (ICUT(NC).EQ.0) GO TO 210
NLNC=NL(NC)
NHPNC=NHP(NC)
NEW=NHPNC-NEW+1
DO 209 K=1,NEW
KK=KK+1
K1=K
K2=2
209 CONTINUE
CALL LIN2 (VT,WIN,DELTAV,RRATIO,AMIN,DELTA,NEW,-1,NC)
210 CONTINUE
IF (IPLT.EQ.2.OR.IPLT.EQ.3) CALL LINE (VT,WIN,DELTAV,TFL,AMIN,
?WIN1A, WIN2A, 0, 0) CALL PLOT2
C
C STORE LABELS FOR SUMMARY.
C
C SUMRDN (NSS)=RUN
DO 250 K=1,15
SUMADE (NSS,K)=ADENT(K)
250 CONTINUE
500 CONTINUE
IF (ICOR.EQ.1) GO TO 530
C
C OUTPUT PARABOLIC SUMMARY
C
C (THIS SECTION IS SKIPPED IF ICOR=1)
C
C KK=NSS-1
WRITE (*,2)
WRITE (*,6)
DO 525 L=1,6
WRITE (*,65) SUMRDN(L),COF(L),DCOF(L),ZERO(L),SUMADE(L,K),K=1,5
525 CONTINUE
530 CONTINUE
C
C OUTPUT FITTING SUMMARY
C
C (THIS SECTION IS SKIPPED IF IFIT=0)
C
C IF (IFIT.EQ.0) GO TO 550
KR=MSS-1
DO 540 JK=1,MPARM
    J=ORDER(JK)
    WRITE(6,2)
    GO TO(701,702,703,704,705,706,707,708,709,710,711,712,713,714),J
701 WRITE(6,901)
    GO TO 537
702 WRITE(6,902)
    GO TO 537
703 WRITE(6,903)
    GO TO 537
704 WRITE(6,904)
    GO TO 537
705 WRITE(6,905)
    GO TO 537
706 WRITE(6,906)
    GO TO 537
707 WRITE(6,907)
    GO TO 537
708 WRITE(6,908)
    GO TO 537
709 WRITE(6,909)
    GO TO 537
710 WRITE(6,910)
    GO TO 537
711 WRITE(6,911)
    GO TO 537
712 WRITE(6,912)
    GO TO 537
713 WRITE(6,913)
    GO TO 537
714 WRITE(6,914)
537 CONTINUE
    WRITE(6,936)
    DO 540 LL=1,KK
    WRITE(6,845)(SUM(DF,L),LL=1,5)
    WRITE(6,840)(PARM(L,J),DFARM(L,J))
540 CONTINUE
550 CONTINUE
    WRITE(6,2)
STOP
END
FUNCTION = (ALPHA (1) + OFF) / P

END
FUNCTION WW(V)

C SUBPROGRAM TO FIND THE ANGULAR FREQUENCY FROM THE WAVENUMBER

C REAL*8 DV, DW
DV=DBLE(V)
DW=DV*2.50*3.1415927D0*2.997929D10
WW=SMGL(DW)
RETURN
END
SUBROUTINE DRUDE(W,E1,E2,WP,T)

******************************************************************************
SUBROUTINE TO FIND THE REAL(E1) AND IMAGINARY(E2) PARTS OF THE
DIELECTRIC FUNCTION OF A METAL USING THE DRUDE MODEL.
******************************************************************************

WP=PLASMA FREQUENCY
T=RELAXATION TIME
W=FREQUENCY

REAL*8 DW,DWP,DT,DE1,DE2,PA,PFA
DWP=DBLE(W)
DT=DBLE(T)
PA=DWP*DW/(DW*DW+(1.DO/DT)**2)
DE1=1.DO-PA
IF(W)10,10,15
10 CONTINUE
DE2=1.DO
GO TO 16
15 CONTINUE
PFA=1.DO/(DW*DT)
DE2=PFA*PA
E1=SNGL(DE1)
E2=SNGL(DE2)
16 CONTINUE
RETURN
END
SUBROUTINE CHI_EL (IT, F, RLA, RLS, PCI, CLA, CLS, VV, BE1, BE2, EP1, EP2, EPC1, EPC2, EPGLC1, EPGLC2, PRC1, PRC2, PHC1, PHC2, XUC1, XUC2, XGHUC1, XGHUC2) 

C****************************************************************************C
C PROGRAM TO FIND THE ABSORPTION COEFFICIENT OF A SYSTEM OF CLUSTERED SPHERES USING THE MAXWELL GARNETT APPROACH BUT INCLUDING MAGNETIC DIPOLE TERMS.
C THE THEORY IS USED TO FIND THE POLARIZABILITIES OF THE CLUSTERS.
C THE CLUSTER DIAMETERS ARE ASSUMED TO FOLLOW A LOG-NORMAL DISTRIBUTION.
C THE METAL IS ASSUMED TO BE THE HOST INSIDE THE CLUSTER.
C*****************************************************************************
C INPUT:
C P = OVERALL FILLING FRACTION
C RLA = AVERAGE OF THE LOG OF THE PARTICLE DIAMETERS IN LN (MICRONS)
C RLS = STANDARD DEVIATION OF THE LOG OF THE PARTICLE DIAMETERS
C PCI = FILLING FRACTION OF METAL INSIDE CLUSTER
C CLA = AVERAGE OF THE LOG OF THE CLUSTER DIAMETERS IN LN (MICRONS)
C CLS = STANDARD DEVIATION OF THE LOG OF THE CLUSTER DIAMETERS
C VV = WAVENUMBER IN CM^-1
C BE1, BE2 = ELECTRIC POLARIZABILITY OF PARTICLE
C EP1, EP2 = ELECTRIC CONSTANT OF BULK MATERIAL
C RLC, RLC2 = DISSIPATIVE DIAMETER OF METAL INSIDE CLUSTER
C EPGLC1, EPGLC2 = ELECTRIC POLARIZABILITY OF CLUSTER
C EPGLC1, EPGLC2 = DIEMETRIC CONSTANT OF CLUSTER
C PRC1, PRC2 = ELECTRIC POLARIZABILITY OF CLUSTER
C PR1, PR2 = DIEMETRIC CONSTANT OF HOST MATERIAL
C PHC1, PHC2 = DIEMETRIC CONSTANT OF CLUSTER
C XUC1, XUC2 = DIEMETRIC CONSTANT OF CLUSTER

C*****************************************************************************
C OUTPUT:
C EP1, EP2 = ELECTRIC POLARIZABILITY OF PARTICLE
C EPGLC1, EPGLC2 = DIEMETRIC CONSTANT OF CLUSTER
C PHC1, PHC2 = DIEMETRIC CONSTANT OF CLUSTER
C PR1, PH2 = MAGNETIC POARIZABILITY OF CLUSTER
C EE1, EE2 = DUMMY
C FLC = ELECTRIC POLARIZABILITY OF CLUSTER
C PRC1, PRC2 = EFFECTIVE DIEMETRIC CONSTANT OF COMPOSITE
C PHC1, PHC2 = EFFECTIVE DIEMETRIC CONSTANT OF COMPOSITE
C XUC1, XUC2 = DIEMETRIC CONSTANT OF CLUSTER
C XGHUC1, XGHUC2 = DUMMY

C****************************************************************************
C DIMENSION VV (IT), BE1 (IT), BE2 (IT), EP1 (IT), EP2 (IT)
C * EPC1 (IT), EPC2 (IT), PHC1 (IT), PHC2 (IT), PRC1 (IT), PRC2 (IT)
C * EE1 (IT), EE2 (IT), EPGLC1 (IT), EPGLC2 (IT)
C * XUC1 (IT), XUC2 (IT), XGHUC1 (IT), XGHUC2 (IT), PR1 (IT), PR2 (IT)
C XGHUC1, XGHUC2 = DUMMY

C*****************************************************************************
C CALCULATE THE ELECTRICAL POLARIZABILITY (EP1, EP2) OF A SPHERE
C*****************************************************************************
C IL1=4, IL2=10, IL3=4, IL4=10, IL5=4, IL6=10
C CALL EPOLEtEP! (IV), EP2 (IT), EP2 (IT)
C*****************************************************************************
C CALL SUBROUTINE TO FIND MAXWELL GARNETT THEORY RESULT FOR THE EFFECTIVE DIEMETRIC CONSTANT OF CLUSTER
C*****************************************************************************
C CALL MAXGARN (EPC1 (IT), EPC2 (IT), EP1 (IT), EP2 (IT), BE1 (IT), BE2 (IT), X1L, X1L2, X1L3)
C*****************************************************************************
C
CALL MACRO (MACRO1 (IA), MACRO2 (IA), MACRO3 (IA))
SUBROUTINE BRUGGERH'S SYMMETRICAL EFFECTIVE MEDIUM THEORY TO
CALL EPHED (EP1, EP2, PH1, PH2, PHC1, PHC2, PCI, PF1, PF2, PC1, PC2,
DIELECTRIC CONSTANT OF CLUSTER.
MAGNETIC POLARIZABILITY OF CLUSTER.
EFFECTIVE MAGNETIC PERMEABILITY OF COMPOSITE
EFFECTIVE DIELECTRIC CONSTANT OF COMPOSITE
ALPHA = ABSORPTION COEFFICIENT OF COMPOSITE
DIELECTRIC CONSTANT OF CLUSTER.
EFFECTIVE ELECTRIC POLARIZABILITY OF COMPOSITE.
CALL SDBRODTINF TO FIND MAXWELL GARNETT THEORY RESULT FOR THE
EFFECTIVE DIELECTRIC CONSTANT OF COMPOSITE

CALL MAIGAR (EMGC1 (IV) ,EMGC2 (IV) ,EPC1 (IV) ,EPC2 (IV) ,HE1 (IV) ,HE2 (IV) ,
PCL)

CALL MAIGAR (XG01 (IV) ,XG02 (IV) ,PH1 (IV) ,PH2 (IV) ,1.,0.,PCL)

CALL ABSOR (EMGC1 (IV) ,EMGC2 (IV) ,XG01 (IV) ,XG02 (IV) ,VV (IV) ,
*ALPHA (IV))
RETURN
END
SUBROUTINE CHIE (IV, F, A, FC1, CL, IV, BP1, BF2, BE1, BE2, EP1, EP2, ENG1, ENG2, PH1, PH2, PH1, PH2, IU1, IU2, IgHU1, IgHU2, ALPHA, SALPHA, TPC1, TPC2, ENG1C, ENG2C, PRC1, PRC2, PRC1, PRC2, XOC1, XOC2, XGHUC1, XGHUC2)

PROGRAM TO FIND THE ABSORPTION COEFFICIENT OF A SYSTEM OF CLUSTERED SPHERES USING THE MAXWELL GARNETT APPROACH BUT INCLUDING MAGNETIC DIPOLE TERMS.

THE THEORY IS USED TO FIND THE POLARIZABILITIES OF THE CLUSTERS.

THE METAL IS ASSUMED TO BE THE HOST INSIDE THE CLUSTER.

INPUT:
F
-FI
FCI
-FCL
C1
-C1
(BE1, BE2)
-HE1, HE2)

OUTPUT:
-EP1, EP2)
-EP1, EP2)
(TPC1, TPC2)
-PRC1, PRC2)

DIMENSION IV [1], BE1 [1], BE2 [1], EP1 [1], EP2 [1];
*ENG1 [1], ENG2 [1], PH1 [1], PH2 [1], PH1 [1], PH2 [1],
*XU1 [1], XU2 [1], IgHU1 [1], IgHU2 [1],
*ALPHA [1], SALPHA [1],
*EP1C [1], TPC2 [1], PRC1 [1], PRC2 [1],
*ENG1C [1], ENG2C [1], PRC1 [1], PRC2 [1],
*PCL [Y] = PCL
*PY = -F

CALL EPOLE (EP1 [IV], EP2 [IV], 1, 0, BE1 [IV], BE2 [IV], XU1, XU2, XU3)

CALL HAXGAR (ENG1 [IV], ENG2 [IV], EP1 [IV], EP2 [IV], BE1 [IV], BE2 [IV], PY)

CALL HIEPOL (PCLC [IV], TPC2 [IV], PRC1 [IV], PRC2 [IV], 1, 0, ENG1C [IV], ENG2C [IV])

CALL RIEPOL (ENG1 [IV], ENG2 [IV], PFI [IV], PH1 [IV], PH2 [IV], ENG1 [IV], ENG2 [IV])

CALCULATE THE ELECTRICAL POLARIZABILITY (EP1, EP2) OF A SPHERE

CALCULATE THE EFFECTIVE ELECTRIC POLARIZABILITY (EP1, EP2) OF A SPHERE

CALL HAXGAR (ENG1 [IV], ENG2 [IV], EP1 [IV], EP2 [IV], BE1 [IV], BE2 [IV], PY)

CALL HIEPOL (PCLC [IV], TPC2 [IV], PRC1 [IV], PRC2 [IV], 1, 0, ENG1C [IV], ENG2C [IV])

CALL RIEPOL (ENG1 [IV], ENG2 [IV], PFI [IV], PH1 [IV], PH2 [IV], ENG1 [IV], ENG2 [IV])
CALL SUBROUTINE TO FIND MAXWELL GARNETT THEORY RESULT FOR THE EFFECTIVE DIELECTRIC CONSTANT OF COMPOSITE.

CALL MAIGAR(EMGC1(IV),EMGC2(IV),EPC1(IV),EPC2(IV),HE1(IV),HE2(IV),PCL)

CALL MAIGAR(XGMC1(IV),XGMC2(IV),XGMC1(IV),XGMD2(IV),TV,IV,ALPHA(IV))

CALL ABSOR(EMGC1(IV),EMGC2(IV),XGMC1(IV),XGMD2(IV),TV,IV,ALPHA(IV))
RETURN
END
SUBROUTINE ECUI (IV, A, FC1, CL, VV, BE1, BE2, HE1, HE2, EP1, EP2, EMG1, EMG2, PR1, PR2, PM1, PM2, T1, T2, XG01, XG02, ALPHA, SALPHA, EPC1, EPC2, EMGC1, EMGC2, PRC1, PRC2, PHC1, PHC2, XUC1, XUC2, XGH01, XGH02, XGMC1, XGMC2)

**PROGRAM TO FIND THE ABSORPTION COEFFICIENT OF A SYSTEM OF CLUSTERED SPHERES USING BROUGGERHAN'S SYMMETRICAL EFFECTIVE MEDIUM THEORY TO CALCULATE THE DIELECTRIC CONSTANT OF THE SPHERES AND THE MAXWELL GARNETT APPROACH TO FIND THE ELECTRICAL AND MAGNETIC PROPERTIES OF THE COMPOSITE.**

**INPUT:**
- **F** = OVERALL FILLING FRACTION
- **A** = PARTICLE DIAMETER IN CM
- **FCI** = CLUSTER DIAMETER IN CM
- **VV** = WAVELENGTH IN CM
- **BE1, BE2** = DIELECTRIC CONSTANT OF BULK MATERIAL
- **HE1, HE2** = DIELECTRIC CONSTANT OF HOST MATERIAL

**OUTPUT:**
- **FP, PP** = DWMMY
- **EMG1, EMG2** = DIELECTRIC CONSTANT OF CLUSTER
- **PRC1, PRC2** = EFFECTIVE DIELECTRIC CONSTANT OF COMPOSITE
- **PHC1, PHC2** = EFFECTIVE MAGNETIC PERMEABILITY OF COMPOSITE
- **EPC1, EPC2** = ELECTRIC POLARIZABILITY OF CLUSTER
- **EMGC1, EMGC2** = EFFECTIVE ELECTRIC POLARIZABILITY OF COMPOSITE

**DIMENSION IV (IV), BE1 (IV), BE2 (IV), EP1 (IV), EP2 (IV),
* FG1 (IV), FG2 (IV), PM1 (IV), PM2 (IV),
* XG01 (IV), XG02 (IV),
* ALPHA (IV), SALPHA (IV),
* EPC1 (IV), EPC2 (IV), EMGC1 (IV), EMGC2 (IV),
* PRC1 (IV), PRC2 (IV), PHC1 (IV), PHC2 (IV),
* XUC1 (IV), XUC2 (IV), XG01 (IV), XG02 (IV),
* ALPHA (IV), SALPHA (IV),
* EPC1 (IV), EPC2 (IV), EMGC1 (IV), EMGC2 (IV),
* PRC1 (IV), PRC2 (IV), PHC1 (IV), PHC2 (IV),
* XUC1 (IV), XUC2 (IV), XG01 (IV), XG02 (IV),
* XGH01 (IV), XGH02 (IV), XGMC1 (IV), XGMC2 (IV),**

**CALL SUBROUTINE TO FIND BROUGGERHAN'S SYMMETRICAL EFFECTIVE MEDIUM RESULT FOR THE EFFECTIVE DIELECTRIC CONSTANT OF THE CLUSTER.**

**CALL EFFHED (EMG1 (IV), EMG2 (IV), BE1 (IV), BE2 (IV), 1, 0, FC1, PV) **

**CALL HIEPOL (EPC1 (IV), EPC2 (IV), EMGC1 (IV), EMGC2 (IV),
PRC1 (IV), PRC2 (IV), PHC1 (IV), PHC2 (IV),
XUC1 (IV), XUC2 (IV), XGMC1 (IV), XGMC2 (IV), HE1 (IV), HE2 (IV),**

**CALL MAXGAR (EMGC1 (IV), EMGC2 (IV), EPC1 (IV), EPC2 (IV), HE1 (IV), HE2 (IV),**
FIND THE MAXWELL-GARNETT RESULT FOR THE EFFECTIVE MAGNETIC PERMEABILITY ($\mu_1$, $\mu_2$) OF COMPOSITE.

CALL MAIGAB ($\mu_1$(IV), $\mu_2$(IV), $\mu_{11}$(IV), $\mu_{12}$(IV), 1., 0., FCL)

FIND THE ABSORPTION COEFFICIENT FROM THE EFFECTIVE ELECTRICAL AND MAGNETIC PROPERTIES OF THE COMPOSITE.

CALL ABSOR($\mu_{11}$, $\mu_{12}$, $\mu_{01}$, $\mu_{02}$, $\alpha$(IV))

RETURN
END
CALL EPOL(EPC1(IV),EPC2(IV),EMG1(IV),EMG2(IV),HE1(IV),HE2(IV), XL1,XL2,XL3)

CALL SUBROUTINE TO FIND MAXWELL GARNETT THEORY RESULT FOR THE EFFECTIVE DIELECTRIC CONSTANT OF COMPOSITE

CALL MAIGAR(EMGC1(IV),EMGC2(IV),EPC1(IV),EPC2(IV),HE1(IV),HE2(IV), PCL)

CALL PROP(V(IV),EMG1(IV),EMG2(IV),1.,0.,PF1(IV),PR2(IV))

CALL HPOLE(PH1(IV),PH2(IV),PF1(IV),PR2(IV),CL)

CALL INDPID(XU1(IV),XU2(IV),PB1(IV),PH2(IV))

CALL MAIGAR(XGMU1(IV),XGMU2(IV),PM1(IV),PM2(IV),1.,0.,FCL)

CALL ABSOR(EMGC1(IV),EMGC2(IV),XGMU1(IV),XGMU2(IV),V(IV), ALPHA(IV))

RETURN
END
SUBROUTINE EHCLUS (IV, F, FCT, CL, VV, BE1, BE2, E1, E2, EP1, EP2,
  ENG1, ENG2, PR1, PR2, PR, I1, I2, IOM, IGMC, ALPHA, SALPHA,
  EPC1, EPC2, EMGC1, EMGC2, PRC1, PRC2, PRMC1, PRMC2, XUC1, XUC2, IGMUC1, IGMUC2)

********* PROGRAM TO FIND THE ABSORPTION COEFFICIENT OF A SYSTEM OF CLUSTERED SPHERES USING THE BRUGGMAN'S SYMMETRICAL EFFECTIVE MEDIUM THEORY APPROACH TO FIND THE PROPERTIES OF THE CLUSTER AND THE MAXWELL GARNETT THEORY TO FIND THE PROPERTIES OF THE COMPOSITE. THE SIMPLE THEORIES ARE USED TO FIND THE POLARIZABILITIES THE METAL IS ASSUMED TO BE THE HOST INSIDE THE CLUSTER.

INPUT:
  F = OVERALL FILLING FRACTION
  FCT = PARTICLE DIAMETER IN CM
  CL = CLUSTER DIAMETER IN CM
  VV = WAVELENGTH IN CM
  (BE1, BE2) = DIELCTRICAL CONSTANT OF BULK MATERIAL
  (HE1, HE2) = DIELCTRICAL CONSTANT OF HOST MATERIAL

OUTPUT:
  (EP1, EP2) = EFFECTIVE DIELECTRIC CONSTANT OF COMPOSITE
  (ENG1, ENG2) = EFFECTIVE ELECTRIC POLARIZABILITY CLUSTER
  (PR1, PR2) = PROPAGATION CONSTANT INSIDE CLUSTER
  (PRC1, PRC2) = DIELCTRICAL CONSTANT OF CLUSTER
  (PRMC1, PRMC2) = DIELCTRICAL CONSTANT OF HOST MATERIAL
  (XUC1, XUC2) = DIELCTRICAL CONSTANT OF HOST MATERIAL

DIMENSION VV(1), BE1(1), BE2(1), E1(1), E2(1),
  I1(1), I2(1), IOM(1), IGMC(1),
  ALPHA(1), SALPHA(1),
  ENG1(1), ENG2(1), PR1(1), PR2(1), PR(1),
  IOM(1), IGMC(1),
  EPC1(1), EPC2(1), EMGC1(1), EMGC2(1),
  PRC1(1), PRC2(1), PRMC1(1), PRMC2(1),
  XUC1(1), XUC2(1), IGMUC1(1), IGMUC2(1), HE1(1), HE2(1),
  FC1, FC2, FC3,
  FCL, FCLV, FV, FV0)

CALL SUBROUTINE TO FIND BRUGGMAN'S SYMMETRICAL EFFECTIVE MEDIUM THEORY RESULT FOR THE EFFECTIVE DIELECTRIC CONSTANT OF CLUSTER.

CALL EFFRED (ENG1(IV), ENG2(IV), BE1(IV), BE2(IV), E1(IV), E2(IV), EP1(IV), EP2(IV),
  PR1(IV), PR2(IV), PR(IV), I1(IV), I2(IV), IOM(IV), IGMC(IV),
  ALPHA(IV), SALPHA(IV),
  EPC1(IV), EPC2(IV), EMGC1(IV), EMGC2(IV),
  PRC1(IV), PRC2(IV), PRMC1(IV), PRMC2(IV),
  XUC1(IV), XUC2(IV), IGMUC1(IV), IGMUC2(IV), HE1(IV), HE2(IV),
  XL1, XL2, XL3)

CALL SUBROUTINE TO FIND MAXWELL GARNETT THEORY RESULT FOR THE EFFECTIVE DIELECTRIC CONSTANT OF COMPOSITE.
CALL RAX GIB (EBGC1 (IT), EBGC2 (IT), EPC1 (IT), EPC2 (IV), RE1 (IT), HE2 (IT), PFCL)

C CALCULATE PROPAGATION CONSTANT (PR1, PR2) INSIDE THE CLUSTERS

C

CALL PROP (V (IV), ENG1 (IT), ENG2 (IV), 1., 0., PR1 (IT), PR2 (IT))

C

C

C CALCULATE THE MAGNETIC POLARIZABILITY (PM1, PM2) OF THE CLUSTERS

C

CALL HPOLE (PH1 (IV), PH2 (IV), PE1 (IV), PR2 (IV), CL)

C

C

C CALCULATE THE MAGNETIC PERMEABILITY (XU1, XU2) OF THE CLUSTERS

C

CALL INDHU (XU1 (IV), XU2 (IV), PH1 (IV), PH2 (IT))

C

C FIND THE MAXWELL GARNETT RESULT FOR THE EFFECTIVE MAGNETIC

C AND ELECTRICAL PROPERTIES OF THE COMPOSITE

C

CALL MAXGAR (ENGC1 (IV), ENGC2 (IV), RPC1 (IV), RPC2 (IV), RE1 (IV), RE2 (IV), PFCL)

C

C

C FIND THE ABSORPTION COEFFICIENT FROM THE EFFECTIVE ELECTRICAL

C AND MAGNETIC PROPERTIES OF THE COMPOSITE

C

CALL ABSOR (ENGC1 (IV), ENGC2 (IV), XGMU1 (IV), XGMU2 (IV), VV (IV), *ALPHA (IT))

RETURN

END
SUBROUTINE IHIFL (TV, F, I, FLS, FCI, CLA, CLS, VV, BE1, BE2, HE1, HE2, EP1, EP2, ENG1, ENG2, PR1, PR2, PM1, PM2, XU1, XU2, XGMU1, XGMU2, ALPHA, SALPHA, TEP1, TEP2, ENG1, ENG2, PR1, PR2, PM1, PM2, XOC1, XOC2, XGMUC1, XGMUC2)

C PROGRAM TO FIND THE ABSORPTION COEFFICIENT OF A SYSTEM OF ISOLATED SPHERES USING THE MAXWELL GARNETT APPROACH BUT INCLUDING MAGNETIC DIPOLE TERMS.
C MIX THEORY IS USED TO FIND THE POLARIZABILITIES.
C THE PARTICLE DIAMETERS ARE ASSUMED TO FOLLOW A LOG-NORMAL DISTRIBUTION.

INPUT:
FLA = OVERALL FILLING FRACTION
FLS = STANDA)RD DEVIATION OF THE LOG OF THE PARTICLE DIAMETERS IN LN (MICRONS)
FCI = FILLING FRACTION OF METAL INSIDE CLUSTER
CLS = STANDARD DEVIATION OF THE LOG OF THE CLUSTER DIAMETERS IN LN (MICRONS)
VV = WAVENUMBER IN CM-1
(PE1,BE2) = DIELECTRIC CONSTANT OF BULK MATERIAL
(RE1,HE2) = DIELECTRIC CONSTANT OF HOST MATERIAL

OUTPUT:
(EP1,EP2) = ELECTRIC POLARIZABILITY OF PARTICLE
(ENG1,ENG2) = ELECTRIC POLARIZABILITY OF COMPOSITE
(PR1,PR2) = MAGNETIC POLARIZABILITY OF PARTICLES
(PR1,PR2) = MAGNETIC POLARIZABILITY OF COMPOSITE
(XGMU1, XGMU2) = EFFECTIVE MAGNETIC PERMEABILITY OF COMPOSITE
ALPHA = ABSORPTION COEFFICIENT OF COMPOSITE
SALPHA = DUMMY

DIMENSION VV(1), BE1(1), BE2(1), EP1(1), EP2(1),
(ENG1,ENG2, PR1, PR2, PM1, PM2,)
(XU1, XU2, XGMU1, XGMU2,)
(ALPHA, SALPHA,)
(EP1, EP2, ENG1, ENG2, PR1, PR2, PM1, PM2,)
(XOC1, XOC2, XGMUC1, XGMUC2,)

CALL LOGDIS (EP1(1), EP2(1), PM1(1), PM2(1), BE1(1), BE2(1),
(RE1, RE2),, VV(1), VV(1), FLA, FLS)

CALL SUBROUTINE TO FIND MAXWELL GARNETT THEORY RESULT FOR THE EFFECTIVE DIELECTRIC CONSTANT OF COMPOSITE

CALL MAIGAR (ENG1, ENG2, VV, EP1(1), EP2(1), RE1(1), RE2(1), F)
FIND THE MAXWELL GARNETT RESULT FOR THE EFFECTIVE MAGNETIC
PERMEABILITY (IMG1, IMG2)

CALL MAGAR (IMG1, IMG2, PR1, PR2, 1, 0, P)

FIND THE ABSORPTION COEFFICIENT FROM THE EFFECTIVE ELECTRICAL
AND MAGNETIC PROPERTIES OF THE COMPOSITE

CALL ABSOR (ENG1, ENG2, IMG1, IMG2, WV, ALPHA)
RETURN
END
SUBROUTINE IBIEFIV, F, A, PCICL, YV, BE1, BE2, HE1, HE2, EP1, EP2, EMG1, EMG2, PH1, PH2, PR1, PR2, XG1, XG2, XM1, XM2, ALPHA, SALPHA, EPC1, EPC2, EMGC1, EMGC2, PHC1, PHC2, PRC1, PRC2, XOC1, XOC2, XMOC1, XMOC2)

PROGRAM TO FIND THE ABSORPTION COEFFICIENT OF A SYSTEM OF ISOLATED SPHERES USING THE MAXWELL GARNETT APPROACH BUT INCLUDING MAGNETIC DIPOLE TERMS.

MIE THEORY IS USED TO FIND THE POLARIZABILITIES.

INPUT:

- \( F \) = OVERALL FILLING FRACTION
- \( \text{PCICL} \) = PARTICLE DIAMETER IN CM
- \( \text{YV} \) = WAVELENGTH IN CM
- \( \text{BE1}, \text{BE2} \) = DIELECTRIC CONSTANT OF BULK MATERIAL
- \( \text{HE1}, \text{HE2} \) = DIELECTRIC CONSTANT OF HOST MATERIAL

OUTPUT:

- \( \text{EP1}, \text{EP2} \) = ELECTRIC POLARIZABILITY OF PARTICLE
- \( \text{PR1}, \text{PR2} \) = DUMMY
- \( \text{PH1}, \text{PH2} \) = MAGNETIC POLARIZABILITY OF PARTICLES
- \( \text{ALPHA} \) = ABSORPTION COEFFICIENT OF COMPOSITE
- \( \text{EMGC1}, \text{EMGC2} \) = EFFECTIVE MAGNETIC PERMUTATION OF COMPOSITE
- \( \text{XXX1}, \text{XXX2} \) = DUMMY

CALCULATE THE ELECTRICAL (EP1, EP2) AND MAGNETIC (PH1, PH2) POLARIZABILITY OF A SPHERE.

CALL HIEPOL (EP1(1), EP2(1), PH1(1), PH2(1), BE1(1), BE2(1), HE1(1), HE2(1), F)

CALL SUBROUTINE TO FIND MAXWELL GARNETT THEORY RESULT FOR THE EFFECTIVE DIELECTRIC CONSTANT OF COMPOSITE.

CALL HAXGAR (EMG1(1), EMG2(1), PH1(1), PH2(1), XG1(1), XG2(1), XM1(1), XM2(1), EMGC1(1), EMGC2(1), ALPHA(1), SALPHA(1), XOC1(1), XOC2(1), XMOC1(1), XMOC2(1), FCL, PCI, PCLY = 1, PCL, FV = 1, PCI, FVO = 1, -F)

CALCULATE THE EFFECTIVE DIELECTRIC CONSTANT OF COMPOSITE.

CALL HAXGAR (EMG1(1), EMG2(1), EP1(1), EP2(1), HE1(1), HE2(1), F)

FIND THE MAXWELL GARNETT RESULT FOR THE EFFECTIVE MAGNETIC PERMUTATION (XMOC1, XMOC2).

CALL HAXGAR (XMOC1(1), XMOC2(1), PH1(1), PH2(1), XUC1(1), XUC2(1), F)

AA = A^2

CALL HIEPOL (EP1(IV), EP2(IV), PH1(IV), PH2(IV), BE1(IV), BE2(IV), HE1(IV), HE2(IV), F)

THE EFFECTIVE DIELECTRIC CONSTANT OF COMPOSITE.

CALL HAXGAR (EMG1(IV), EMG2(IV), EP1(IV), EP2(IV), HE1(IV), HE2(IV), F)

FIND THE MAXWELL GARNETT RESULT FOR THE EFFECTIVE MAGNETIC PERMUTATION (XMOC1, XMOC2).

CALL HAXGAR (XMOC1(IV), XMOC2(IV), PH1(IV), PH2(IV), F)
C FIND THE ABSORPTION COEFFICIENT FROM THE EFFECTIVE ELECTRICAL
AND MAGNETIC PROPERTIES OF THE COMPOSITE

CALL ABSOR(ENG1(IV),ENG2(IV),IGH1(IV),IGM2(IV),VW(IV),ALPHA(IV))
RETURN
END
**SUBROUTINE EDDY**

**INPUT:**
- \( \text{IT} \) = OVERALL FILLING FRACTION
- \( \text{FCI} \) = PARTICLE DIAMETER IN CM
- \( \text{CL} \) = CLUSTER DIAMETER IN CM
- \( \text{VV} \) = WAVE NUMBER IN CM\(^{-1} \)
- \( \{\text{BE1}, \text{BE2}\} \) = ELECTRIC POLARIZABILITY OF PARTICLE
- \( \{\text{EHG1}, \text{EHG2}\} \) = ELECTRIC POLARIZABILITY OF COMPOSITE
- \( \{\text{PR1}, \text{PR2}\} \) = PROPAGATION CONSTANT INSIDE PARTICLES
- \( \{\text{PRC1}, \text{PRC2}\} \) = MAGNETIC POLARIZABILITY OF PARTICLES
- \( \{\text{XGMD1}, \text{XGMD2}\} \) = EFFECTIVE MAGNETIC PERMEABILITY OF COMPOSITE
- \( \text{ALPHA} \) = ABSORPTION COEFFICIENT OF COMPOSITE

**OUTPUT:**
- \( \{\text{EP1}, \text{EP2}\} \) = ELECTRIC POLARIZABILITY OF PARTICLE
- \( \{\text{EP1}, \text{EP2}\} \) = ELECTRIC POLARIZABILITY OF COMPOSITE
- \( \{\text{PR1}, \text{PR2}\} \) = PROPAGATION CONSTANT INSIDE PARTICLES
- \( \{\text{PRC1}, \text{PRC2}\} \) = MAGNETIC POLARIZABILITY OF PARTICLES
- \( \{\text{XGMD1}, \text{XGMD2}\} \) = EFFECTIVE MAGNETIC PERMEABILITY OF COMPOSITE

**PROGRAM TO FIND THE ABSORPTION COEFFICIENT OF A SYSTEM OF ISOLATED SPHERES USING THE MAXWELL GARNETT APPROACH BUT INCLUDING MAGNETIC DIPOLE TERMS.**

**THE VACUUM IS ASSUMED TO BE THE HOST INSIDE THE COMPOSITE.**

**THE SIMPLE THEORIES ARE USED TO FIND THE POLARIZABILITIES.**

**INPUT:**
- \( \text{VV} \) = WAVE NUMBER IN CM\(^{-1} \)
- \( \text{ALPHA} \) = ABSORPTION COEFFICIENT OF COMPOSITE

**OUTPUT:**
- \( \{\text{EP1}, \text{EP2}\} \) = ELECTRIC POLARIZABILITY OF PARTICLE
- \( \{\text{EP1}, \text{EP2}\} \) = ELECTRIC POLARIZABILITY OF COMPOSITE

**CALCULATE THE ELECTRICAL POLARIZABILITY (EP1, EP2) OF A SPHERE**

**CALL EPOLLE (EP1(IV), EP2(IV), BE1(IV), BE2(IV), EH1(IV), EH2(IV), XL1, XL2, XL3)**

**CALL SUBROUTINE TO FIND MAXWELL GARNETT THEORY RESULT FOR THE COMPOSITE**

**CALL HAXGAR (EHG1(IV), EHG2(IV), EP1(IV), EP2(IV), BE1(IV), BE2(IV), P)**

**CALL PROP (VV(IV), BE1(IV), BE2(IV), 1.0, PR1(IV), PR2(IV))**
**CALCULATE THE MAGNETIC POLARIZABILITY \((\mathbf{PM}_1, \mathbf{PM}_2)\) OF THE MATERIAL.**

CALL HPOLE \((\mathbf{PM}_1(IV), \mathbf{PM}_2(IV), \mathbf{PR}_1(IV), \mathbf{PR}_2(IV), A)\)

**CALCULATE THE INDUCED MAGNETIC PERMEABILITY \((\mathbf{XU}_1, \mathbf{XU}_2)\) OF THE PARTICLES.**

CALL INDMO \((\mathbf{XU}_1(IV), \mathbf{XU}_2(IV), \mathbf{PR}_1(IV), \mathbf{PR}_2(IV))\)

**FIND THE MAXWELL GARNETT RESULT FOR THE EFFECTIVE MAGNETIC PERMEABILITY \((\mathbf{XGM}_1, \mathbf{XGM}_2)\)**

CALL MAXGAR \((\mathbf{XGM}_1(IV), \mathbf{XGM}_2(IV), \mathbf{PM}_1(IV), \mathbf{PM}_2(IV), 1.0, F)\)

**FIND THE ABSORPTION COEFFICIENT FROM THE EFFECTIVE ELECTRICAL AND MAGNETIC PROPERTIES OF THE COMPOSITE**

CALL ABSOR \((\mathbf{PM}_1(IV), \mathbf{PM}_2(IV), \mathbf{XGM}_1(IV), \mathbf{XGM}_2(IV), \mathbf{V}_1(IV), \mathbf{ALPHA}(IV))\)

RETURN
END
SUBROUTINE EDDY (IV, P, A, PCI, CL, VV, BE1, BE2, HE1, HE2, EP1, EP2,
TENG1, ENG2, PB1, PB2, PR1, PR2, XU1, XU2, IGM1, IGM2, ALPH1, SALPH1,
EP1C1, EP2C2, ENG1C1, PR1C1, PR2C2, PH1C1, PH2C1, XUC1, XUC2, IGMUC1, IGMUC2)

C**********************************************************************
C PROGRAM TO FIND THE ABSORPTION COEFFICIENT OF A SYSTEM OF ISOLATED
Spheres using Bruggeman's Symmetrical Effective Medium Theory
APPROACH BUT INCLUDING MAGNETIC DIPOLE TERMS.
THE SIMPLE THEORIES ARE USED TO FIND THE POLARIZABILITIES

INPUT:
  F  = OVERALL FILLING FRACTION
  A  = PARTICLE DIAMETER IN CM.
  PCI = FILLING FRACTION OF METAL INSIDE CLUSTER
  CL = CLUSTER DIAMETER IN CM.
  VV = AVENUMBER IN CM^-1
  (BE1, BE2) = DIELECTRIC CONSTANT OF BULK MATERIAL
  (HE1, HE2) = DIELECTRIC CONSTANT OF HOST MATERIAL

OUTPUT:
  (EP1, EP2) = DUMMY
  (ENG1, ENG2) = DIELECTRIC CONSTANT OF COMPOSITE
  (PR1, PR2) = MAGNETIC POLARIZABILITY OF PARTICLES
  (PH1, PH2) = EFFECTIVE MAGNETIC PERMEABILITY OF COMPOSITE
  ALPHA = ABSORPTION COEFFICIENT OF COMPOSITE

DIMENSION VV(1), BE1(1), BE2(1), EP1(1), EP2(1),
* ENG1(1), ENG2(1), PR1(1), PR2(1), PH1(1), PH2(1),
* XU1(1), XU2(1), IGM1(1), IGM2(1),
* ALPH1(1), SALPH1(1),
* ENG1C1(1), ENG2C2(1), PR1C1, PR2C2(1), PH1C1, PH2C2(1),
* XUC1(1), XUC2(1), IGMUC1(1), IGMUC2(1),
* FCL=P/PCI
* FCLV=1.-FCL
* FV=1.-PCI
* FVO=1.-F

CALL EFFMED (ENG1IV, ENG2IV, BE1IV, BE2IV, HE1IV, HE2IV, F, FVO)

CALCULATE PROPAGATION CONSTANT (PR1, PR2) INSIDE THE PARTICLES

CALL PROP (VVIV, BE1IV, BE2IV, 1., 0., PR1IV, PR2IV)

CALCULATE THE MAGNETIC POLARIZABILITY (PR1, PR2) OF THE PARTICLES.

CALL MPOLE (PR1IV, PR2IV, PB1IV, PB2IV, A)

CALCULATE THE INDUCED MAGNETIC PERMEABILITY (XU1, XU2) OF THE
PARTICLES.
CALL INDMU (XU1(IV),XU2(IV),PM1(IV),PM2(IV))

FIND BRUGGERMAN'S SYMMETRICAL EFFECTIVE MEDIUM THEORY RESULT FOR
THE EFFECTIVE MAGNETIC PERMEABILITY (IGN1,IGN2) OF THE COMPOSITE

CALL EFFMED(IGN1(IV),IGN2(IV),XU1(IV),XU2(IV),L..O..F,P,FV0)

FIND THE ABSORPTION COEFFICIENT FROM THE EFFECTIVE ELECTRICAL
AND MAGNETIC PROPERTIES OF THE COMPOSITE

CALL ABSOR(EMG1(IV),EMG2(IV),IGN1(IV),IGN2(IV),VV(IV),ALPHA(IV))

RETURN
END
SUBROUTINE P B O P (V, E1, E2, XNU1, XNU2, PR1, PR2)

SUBROUTINE TO CALCULATE THE PROPAGATION CONSTANT
INSIDE A MATERIAL.

(P1, E2) = DIELECTRIC CONSTANT
(INU1, INU2) = MAGNETIC PERMEABILITY
(PR1, PR2) = PROPAGATION CONSTANT

******************************************************************************

C

******************************************************************************

COMPLEX*16 DCHPLX, E, XNU, PR, CONST, CDSQRT, AR
REAL*8 DE1, DE2, DNU1, DNU2, CO
REAL*8 EPFR(2)
EQUIVALENCE (EPFR(1), PR)

E = DCHPLX (DE1, DE2)
A = E*XNU

PB = CONST*CDSQRT (AR)
PR1 = SNGL (EPFR (1))
PR2 = SNGL (EPFR (2))
RETURN
END
SUBROUTINE EPOLE (EP1,EP2,EB1,EB2,EM1,EM2,XL1,XL2, XL3)

*****************************************************************************

SUBROUTINE TO CALCULATE THE ELECTRICAL POLARIZABILITY OF AN
ELLIPSOID USING THE QUASI-STATIC APPROXIMATION.

{EP1,EP2} = ELECTRICAL POLARIZABILITY
{EB1,EB2} = DIELECTRIC CONSTANT OF ELLIPSOID
{EM1,EM2} = DIELECTRIC CONSTANT OF MATERIAL SURROUNDING ELLIPSOID

XL1, XL2, XL3 = DEPOLARIZATION FACTORS FOR ELLIPSOID
*****************************************************************************

COMPLEX*16 CMPLX, EP1,EB1,EM1,CONST1,CONST2,CONST3
REAL*8 EPFR(2), XL(3)
REAL*8 EP,PI,DL1,DL2,DL3,DEM1,DEM2,DEP1,DEP2
EQUIVALENCE (EPFR(1), EP1)
DL1=DBLE(XL1)
DL2=DBLE(XL2)
DL3=DBLE(XL3)
DEM1=DBLE(EM1)
DEM2=DBLE(EM2)
DEP1=DBLE(EB1)
DEP2=DBLE(EB2)
XL(1)=DL1
XL(2)=DL2
XL(3)=DL3
EBB=DCMPLX(DEP1,DEP2)
EMM=DCMPLX(DEM1,DEM2)
EPF=DCMPLX(0.0D0,0.0D0)
PI=4.0D0*3.1415927D0
DO 10 K=1,3
CONST1=EBB-EMM
CONST2=DCMPLX(PI,0.0D0)*EMM*DCMPLX(XL(K),0.0D0)*CONST1
CONST3=DCMPLX(EP,F,0.0D0)*CONST1/CONST2
EPF=EPF+CONST3
10 CONTINUE
EP1=SNGL(EPFR(1))
EP2=SNGL(EPFR(2))
RETURN
END
SUBROUTINE MPOLE (PM1, PM2, PR1, PR2, A)

C-------------------------------------------------------------
C SUBROUTINE TO FIND THE MAGNETIC POLARIZABILITY OF A SPHERE
C USING LANDAU AND LIFSHITZ'S SOLUTION.
C
C INPUT:
C (PR1, PR2) = PROPAGATION CONSTANT OF FIELD INSIDE SPHERE IN CM-1
C A = DIAMETER OF SPHERE IN CM
C
C OUTPUT:
C (PM1, PM2) = MAGNETIC POLARIZABILITY OF SPHERE
C
C-------------------------------------------------------------

COMPLEX*16 DCMLX, FCDS14, FCDCOS, PR, PH, AAR, CONST1, CONST2, CONST3,
*CONST4, CONST5, AAAR,
*CDABS
PR1=8 DPR1, DPR2, DA, TEST, CO1
PR1=8 EFPR (2)
PR1=DUBLE (PR1)
PR2=DUBLE (PR2)
DA=DBLE (A)
PR=DCMPLX (PR1, PR2)
AAR=DCMPLX (DA, 0.D0)*PR
TEST=CDABS (AAAR)
IF (TEST) 10, 10, 20
10 CONTINUE
AAAR=DCMPLX (1.D-20, 1.D-20)
20 CONTINUE
CO1=3. D0/ (A. D0*3. 1415927D0)
CO1=(-1. D0)*CO1
CONST1=DCMPLX (CO1, 0.D0)
CONST2=DCMPLX (1.D0, 0.D0)
CONST3=DCMPLX (-12.D0, 0.D0)
CONST5 =DCMPLX (2.D0, 0.D0)
AAR=AAR/CONST5
PM=PCDCOS (AAR)/FCDS14 (AAR)
PH=PM*CONST5/AAR
PR=PM*CONST3/AAR
PH=PM*CONST1
PH1=SNGL (EFPR (1))
PH2=SNGL (EFPR (2))
RETURN
END
SUBROUTINE WIEPOL (EP1, EP2, PM1, PM2, EB1, EB2, EM1, EM2, XMUN1, XMUN2,
XMUOU1, XMUOU2, X, R)

SUBROUTINE TO FIND THE ELECTRIC AND MAGNETIC POLARIZABILITIES OF A 
SPHERE USING THE MIE SOLUTION OF A SPHERE IN AN ELECTROMAGNETIC FIELD.

INPUT:

| EB1, EB2 | ELECTRIC CONSTANT OF SPHERE |
| EM1, EM2 | DIELECTRIC CONSTANT OF SURROUNDING MATERIAL |
| XMUN1, XMUN2 | MAGNETIC PERMEABILITY OF SPHERE |
| XMUOU1, XMUOU2 | MAGNETIC PERMEABILITY OF SURROUNDING MATERIAL |
| X, R | WAVE NUMBER IN CM^-1 |

OUTPUT:

| EP1, EP2 | ELECTRIC POLARIZABILITY |
| PM1, PM2 | MAGNETIC POLARIZABILITY |

BREAL8 DEP1, DEP2, DPM1, DPM2, DEM1, DEM2, DMUIN1, DMUIN2,
?DMUOU1, DMUOU2, DY, DR, DBLL, DO, PULL(2)
COMPLE*16 EB, EM, DCMPLX, DCO, AR, CDSORT, EP, PM, SCIN, SCOU, XMUN1,
| XMUOU1, XMUOU2 | CMPLX, XHUIH1, XHUIN2 |
| IHUOU1, IHUOU2 | DBLE (EB1, EB2) |
| DEB1 = DBLE (EB1) |
| DEB2 = DBLE (EB2) |
| DEM1 = DBLE (EM1) |
| DEM2 = DBLE (EM2) |
| DMUIN1 = DBLE (XMUN1) |
| DMUIN2 = DBLE (XMUN2) |
| DMUOU1 = DBLE (XMUOU1) |
| DMUOU2 = DBLE (XMUOU2) |
| DY = DBLE (Y) |
| DR = DBLE (R) |
| EB = DCMPLX (DEB1, DEB2) |
| EM = DCMPLX (DEM1, DEM2) |
| XMUN = DCMPLX (DMUIN1, DMUIN2) |
| XMUOU = DCMPLX (DMUOU1, DMUOU2) |
| DO = 2. DO * 3. 14 * 9. 2 * DDo * DR |
| DCO = DCMPLX (DO, 0.00) |
| AR = EB * XMUN |
| SCIN = DCO * AR |
| SCOU = DCMPLX (AR, 0.00) |
| CALL MIECO (SCIN, SCOU, XMUN, XMUOU, 1, A, B, C, D, XJ, YJ, XH, YH) |
| EP = DCMPLX (12.56637100, 0.00) * JX (2) |
| CPOUL = EP |
| DEPI = PULL (1) |
| DEP2 = PULL (2) |
| EP1 = SINGLE (DEPI) |
| EP2 = SINGLE (DEP2) |
| PM = DCMPLX (1.00, 0.00) |
| PM = DCMPLX (3.00, 0.00) |
| RETURN |
| END |
SUBROUTINE HIECO (SCIN, SCDO, XM0IN, XM0OU, N, A, B, C, D, XJ, YJ, XH, YH)

C SUBROUTINE TO FIND THE MIE SERIES COEFFICIENTS

INPUT:
N=HIGHEST MIE SERIES COEFFICENT TO BE CALCULATED
SCIN=SCATTERING CONSTANT INSIDE SPHERE
SCDO=SCATTERING CONSTANT OUTSIDE SPHERE

OUTPUT:
A=ARRAY OF A MIE SERIES COEFFICIENTS
B=ARRAY OF B MIE SERIES COEFFICENTS
C=ARRAY OF C MIE SERIES COEFFICIENTS
D=ARRAY OF D MIE SERIES COEFFICENTS
XJ=ARRAY OF SPHERICAL BESSEL FUNCTIONS OF THE FIRST KIND WITH
     SCOU AS ARGUMENT
YJ=ARRAY OF SPHERICAL BESSEL FUNCTIONS OF THE FIRST KIND WITH
     SCIN AS ARGUMENT
XH=ARRAY OF SPHERICAL HANKEL FUNCTIONS OF THE FIRST KIND WITH
     SCOU AS ARGUMENT
YH=ARRAY OF SPHERICAL HANKEL FUNCTIONS OF THE FIRST KIND WITH
     SCIN AS ARGUMENT

NOTE: BESSEL FUNCTIONS ARE LABELED BY INTERGERS ONE GREATER THAN IS
      CONVENTIONAL (I.E. J0 IS LABELED J1).

IF CY IS GREATER THAN 138., WHERE CY IS THE ABSOLUTE VALUE OF
      THE IMAGINARY PART OF SCIN, THE VALUES OF C AND D WILL BE
      INCREASED BY A FACTOR OF EXP(CY) WHILE YJ AND YH WILL BE
      REDUCED BY THE SAME FACTOR.

IF CY IS GREATER THAN 138., WHERE CY IS THE ABSOLUTE VALUE OF
      THE IMAGINARY PART OF SCOU, THE VALUES OF C AND D WILL BE
      REDUCED BY A FACTOR OF EXP(CY) WHILE XJ AND XH WILL BE
      REDUCED BY THE SAME FACTOR.

C

COMPLEX*16 PSIX(50), PSIY(50), ETAI(50), ETAY(50):
  * PSIPX(50), PSIPY(50), ETAPI(50), ETAPI(50):
  * XJ(50), YJ(50), XJP(50), YJP(50):
  * C(50), B(50), L(50), D(50), SCIN, SCOU, XM0U, XM0IN:

IMU = (SCIN/SCOU)*(XM0U/XM0IN)
M = 1
CALL CBESS(YJ, YH, YJP, YHP, SCIN, M)
CALL CBESS(XJ, XH, XJP, XHP, SCOU, M)
DO 10 L = 1, N
  K = L+1
  PSIX(K) = SCOU*XJ(K)
  ETAI(K) = SCOU*YJ(K)
  ETAPI(K) = YH(K) + SCOU*XJP(K)
  ETAI(K) = SCIN*YJ(K)
  PSIPX(K) = SCIN*XJ(K)
  PSIPY(K) = YJ(K) + SCIN*YJP(K)
  ETAI(K) = SCIN*YJ(K)
  ETAPI(K) = XH(K) + SCIN*XJP(K)

  A(L) = PSIPY(K) - IMU*PSIX(K)*PSIPX(K)
  A(L) = A(L)/(PSIPY(K)*ETAI(K) - IMU*PSIT(K)*ETAPI(K))
  B(L) = IMU*PSIPX(K)*PSIT(K) - PSIX(K)*PSIPY(K)
  B(L) = B(L)/(PSIT(K)*ETAI(K) - IMU*PSIPX(K)*ETAPI(K))
  C(L) = (PSIX(K) - A(L)*ETAPI(K))/PSIPY(K)
  D(L) = (PSII(K) - B(L)*ETAI(K))/PSIT(K)
10 CONTINUE
RETURN
END
SUBROUTINE CBESS(IJ,IXH,IJP,IXHP,SCOU,N)

SUBROUTINE TO FIND THE SPHERICAL BESSEL AND HANKEL FUNCTIONS OF
THE FIRST KIND AND THEIR DERIVATIVES WITH RESPECT TO THEIR
ARGUMENTS.

XJ = SPHERICAL BESSEL FUNCTIONS OF THE FIRST KIND
XI = SPHERICAL HANKEL FUNCTIONS OF THE FIRST KIND
IJP = DERIVATIVE OF XJ
IXHP = DERIVATIVE OF XI
SCOU = ARGUMENT OF FUNCTIONS
N = HIGHEST ORDER (ACTUALLY, HIGHEST ORDER OF XJ AND XH RETURNED
IS N+1)

FUNCTIONS ARE LABELED BY INTEGERS ONL ORDER GREATER THAN IS
CONVENTIONAL (I.E. J0 IS LABELED J(1))

IF CH IS GREATER THAN 138., WHERE CH IS THE ABSOLUTE VALUE OF
THE IMAGINARY PART OF SCOU, ALL VALUES RETURNED WILL BE REDUCED
BY A FACTOR OF EXP(CH).

REAL*8 CO
COMPLEX*16 DCMLXI, PCSIN, PCDCOS, XJ(51), XI(51), IJP(51), IXHP(51),
?SCOU, CO
XJ(1) = PCSIN(SCOU)/SCOU
XJ(2) = PCSIN(SCOU)/(SCOU**2) - PCDCOS(SCOU)/SCOU
XI(1) = XJ(1) - DCMLXI(0.DO,-1.D0)*PCDCOS(SCOU)/SCOU
XI(2) = XJ(2) + DCMLXI(0.DO,-1.D0)*((FCDCOS(SCOU)/(SCOU**2) +
?FCDSIN(SCOU)/SCOU)
K = N+1
IF (K.LT.3) K = 3
DO 10 L = 3, K
ICO=L-1
CO = DCMLXI(ICO)
CO = 2.D0*CO - 1.D0
CCO = DCMLXI(CO,0.D0)
MK2 = L-2
XJ(L) = XJ(L-1)/SCOU - XJ(L-2)
XI(L) = XI(L-1)/SCOU - XI(L-2)
10 CONTINUE
DO 20 L = 1, N
ICO=L-1
CO = DCMLXI(ICO)
CCO = DCMLXI(CO,0.D0)
IJP(L) = CCO*IXJ(L)/SCOU - IJP(L-1)
IXHP(L) = CCO*IXH(L)/SCOU - IXHP(L-1)
20 CONTINUE RETURN
END
FUNCTION FCDCOS(AR)

FUNCTION FCDCOS(AR) ACTS THE SAME AS CDCOS(AR) IF DABS(DIMAG(AR)) IS LESS THAN OR EQUAL TO 138.

FUNCTION FCDCOS(AR) RETURNS CDCOS(AR) / EXP(DABS(DIMAG(AR))) IF DABS(DIMAG(AR)) IS GREATER THAN 138.

COMPLEX * 16 AR, AR, FCDCOS, FCOSIN, CDOSIN, CDCOS
REAL * 8 RAR(2), DABS, SN, COSIN(2), CH, DCOS, DSIN
EQUIVALENCE (ARR, RAR(1)), (FCOSIN, COSIN(1))
AR = AR
CH = DABS(RAR(2))
IF (CH .LE. (138.0)) GO TO 500
IF (RAR(2) .GE. 0.0) SN = 1.
IF (RAR(2) .LT. 0.0) SN = -1.
COSIN(1) = DCOS(RAR(1)) / 2.0
COSIN(2) = -SN * DSIN(RAR(1)) / 2.0
FCDCOS = FCOSIN
GO TO 600
500 CONTINUE
FCDCOS = CDCOS(AR)
600 CONTINUE
RETURN
END
FUNCTION FCDSIN(AR)

FUNCTION FCDSIN(AR) ACTS THE SAME AS CDSIN(AR) IF DABS(DIMAG(AR)) IS LESS THAN OR EQUAL TO 13B.

FUNCTION FCDSIN(AR) RETURNS CDSIN(AR)/LIP(DABS(DIMAG(AR))) IF DABS(DIMAG(AR)) IS GREATER THAN 13B.

COMPLEX*16 ARR, AR, FCDSIN, PSINE, CDSIN, CDCOS
REAL*8 RAR(2), DABS, SN, SINE(2), CT, DCOS, DSIN
EQUIVALENCE (ARR, RAR(1)), (PSINE, SINE(1))

ARR = AR
CH = DABS(RAR(2))
IF(CH.LE.(13B.D0)) GO TO 500
IF(RAR(2).GE.(0.0))SN = 1.
IF(RAR(2).LT.(0.0))SN = -1.
SINE(1) = DSIN(RAR(1))/2.D0
SINE(2) = SN*DCOS(RAR(1))/2.D0
FCDSIN = PSINE
GO TO 600

500 CONTINUE
FCDSIN = CDSIN(AR)
600 CONTINUE
RETURN
END
SUBROUTINE BAIGAR (EN1, EN2, EP1, EP2, FM1, EM2, F)

C**************************************************************
C SUBROUTINE TO CALCULATE THE MAXWELL GARNETT RESULT FOR THE
C EFFECTIVE DIELECTRIC CONSTANT OF A COMPOSITE MATERIAL.
C (EN1, EN2) = MAXWELL GARNETT DIELECTRIC CONSTANT
C (EP1, EP2) = ELECTRIC POLARIZABILITY OF INCLUSIONS
C (FM1, EM2) = DIELECTRIC CONDUCTIVITY OF HOST
C F = FILLING FRACTION
C**************************************************************
C
COMPLEX*16 DCMPLX, ENG, EP, EM, CF, DEN, XNUM, CTT, CST
REAL*8 DP, DEM1, DEM2, DEP1, DEP2, TT, ST
EQUIVALENCE (EFPR(1), ENG)
DP=DBLE (F)
DEP1=DBLE (EP1)
DEP2=DBLE (EP2)
DEM1=DBLE (EM1)
DEM2=DBLE (EM2)
EP=DCMPLX (DEP1, DEP2)
FM=DCMPLX (DEM1, DEM2)
CF=DCMPLX (DP, 0.0D0)
TT=5.0D0*3.1415927D0/3.0D0
ST=4.0D0*3.1415927D0/3.0D0
CTT=DCMPLX (TT, 0.0D0)
CST=DCMPLX (ST, 0.0D0)
XNUM=DCMPLX (1.0D0, 0.0D0)*CTT*CF*EP
DEN=DCMPLX (1.0D0, 0.0D0)-CST*CF*EP
ENG=EM**XNUM/DEN
EN1=SNGL (EFPR (1))
EN2=SNGL (EFPR (2))
RETURN
END
SUBROUTINE EFFMED(EF1, EF2, FD1, FD2, SD1, SD2, F1, F2)

C-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------
C SUBROUTINE TO CALCULATE BPUGG?MAN'S SYMMETRICAL EFFECTIVE MEDIUM THEORY RESULT FOR THE EFFECTIVE DIELECTRIC CONSTANT OF A TWO COMPONENT COMPOSITE MATERIAL.
C (EF1, EF2) = EFFECTIVE DIELECTRIC CONSTANT
C (FD1, FD2) = EFFECTIVE DIELECTRIC CONSTANT OF FIRST COMPONENT
C (SD1, SD2) = EFFECTIVE DIELECTRIC CONSTANT OF SECOND COMPONENT
C F1 = FILLING FRACTION OF FIRST COMPONENT
C F2 = FILLING FRACTION OF SECOND COMPONENT
C-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------
C COMPLEX*16 DCMPLX, DCMPLXRT, EP, SR, PD, SD, CF1, CF2, GA
REAL*8 DBLE, DBLE1, DEF1, DBF1, DBF2, DSD1, DSD2, DF1, DF2
BEAL*8 DBLE (2)
EQUIVALENCE (EFPR (1), EP)
PD = DBLE (FD1)
DPD1 = DBLE (FD1)
DPD2 = DBLE (FD2)
DFD1 = DBLE (FD1)
DFD2 = DBLE (FD2)
FD = DCMPLX (DF1, DF2)
DF1 = DBLE (F1)
CF1 = DCMPLX (DF1, 0.0)
DF2 = DBLE (F2)
CF2 = DCMPLX (DF2, 0.0)
GA = (DCMPLX (3.0, 0.0) * CF1 - DCMPLX (1.0, 0.0)) * PD
SR = GA * GA + DCMPLX (8.0, 0.0) * PD + SD
SR = DCMPLX (SR)
SR = DCMPLX (SR)
EF = DCMPLX (0.2500, 0.0) * (GA + SR)
TEST = EFFPR (1)
IF (TEST > 100, 101, 101)
100 CONTINUE
101 CONTINUE
DF1 = DBLE (F1)
DF2 = DBLE (F2)
EF1 = EFFPR (1)
EF2 = EFFPR (2)
EF1 = SNGL (DEF1)
EF2 = SNGL (DEF2)
RETURN
END
SUBROUTINE INDMU(XU1,XU2,PM1,PM2)

SUBROUTINE TO FIND THE INDUCED MAGNETIC PERMEABILITY OF A
UNIFORM MOTION MANGNETIZED SPHERE FROM THE INDUCED MAGNETIC
POLARIZABILITY USING THE SIMPLE THEORY.

(XU1,XU2)—INDUCED MAGNETIC PERMEABILITY
(PM1,PM2)—INDUCED MAGNETIC POLARIZABILITY

COMPLEX*16 DCMPLX,XU,PM,CONST1,CONST2,CONST3
REAL*8 DPM1,DPM2,CO
REAL*8 EFPR(2)
EQUIVALENCE (EFPR(1),XU)
DPM1=DOUBLE(PM1)
DPM2=DOUBLE(PM2)
PM=DCMPLX(DPM1,DPM2)
CO=4.0D0*3.141592700
CONST1=DCMPLX(CO,0.D0)
CONST2=DCMPLX(2.0D0,0.D0)
CONST3=DCMPLX(3.0D0,0.D3)
IU=CONST1+CONST2+CONST3*PM
IU=XU/(CONST1-CONST3*PM)
IU1=SGNL(EFPR(1))
IU2=SGNL(EFPR(2))
RETURN
END
SUBROUTINE ABSOR(E1,E2,XU1,XU2,V,ABCO)

C********************************************************************
C SUBROUTINE TO FIND THE ABSORPTION COEFFICIENT FROM THE
C WAVENUMBER (V), THE DIELECTRIC CONSTANT (E1, E2), AND
C THE MAGNETIC PERMEABILITY (XU1, XU2)
C********************************************************************

C COMPLEX*16 DCMPXL,CDSORT,E,XU,AR
REAL*8 DE1,DE2,DXU1,DXU2,DV,DAFCO
REAL*8 EFPR (2)
EQUIVALENCE (EFPR (1),AR)
DE1=DBLE (E1)
DE2=DBLE (E2)
DXU1=DBLE (XU1)
DXU2=DBLE (XU2)
DV=DBLE (V)
E=DCMPXL (DE1,DE2)
XU=DCMPXL (DXU1,DXU2)
AR=E*XU
AR=CDSORT (AR)
DAFCO=3.14159270*D*EFPR (2)
ABCO=SNGL (DAFCO)
RETURN
END
5) Plotting Subroutines
SUBROUTINE PLOT(YDATA, YMIN, DELY, IDATA, XMIN, DELX, XAXIS, MP, *YLABEL, MICHAJ, XLABEL, MICHAJ, JLN, LSY, *RUN, NDECKS, IDENT, NUD, NDENOS, JDENT)

***
THIS SUBPROGRAM PLOTS ARRAY YDATA VERSUS ARRAY XDATA IN A STANDARD FORMAT. SUBPROGRAM IS DESIGNED TO WORK WITH THE VERSATEC PLOTTER.

PAGE SIZE IS 6.5 BY 11 INCHES.

PARAMETERS

YDATA  ARRAY FOR Y AXIS.
YMIN  VALUE WHICH CORRESPONDS TO THE BOTTOM OF THE PLOT.
DELY  INCREMENT WHICH CORRESPONDS TO ONE INCH OF VERTICAL DISTANCE.

NOTE: Y AXIS IS ALWAYS TEN INCHES HIGH.

XDATA  ARRAY FOR X AXIS.
XMIN  VALUE WHICH CORRESPONDS TO THE LEFT EDGE OF THE PLOT.
INCR  INCREMENT WHICH CORRESPONDS TO ONE INCH OF HORIZONTAL DISTANCE.

NOTE: X AXIS IS ALWAYS ONE INCH WIDE.

XAXIS  LENGTH OF X-AXIS, IN INCHES.
MP  NUMBER OF POINTS IN ARRAYS XDATA AND YDATA.

NOTE: MP MUST BE LES THAN NDECKS.

YLABEL  LABEL OF Y AXIS.

XLABEL  LABEL OF X AXIS.

NOTE: XLABEL AND YLABEL ARE READ IN AS LITERAL DATA, ENCLOS MD PARENTHESES.

NOTE: MICHAJ = -MICHAJ THE FIRST TIME TO CAUSE THE AXIS TO BE LABELED ON THE OUTSIDE. MICHAJ = -MICHAJ THE SECOND TIME TO AVOID HAVING THE INTEGER CONSTANT (IE 16) USED AT MICHAJ IN THE CALL TO IMPLOT REDefined AS MISUS THAT INTEGER. THIS IS A FEATURE OF FORTRAN.

LSY  SPECIFIES THE SYMBOL.

USEFUL SYMBOLS: 0:BOX, 1:OCTAGON, 2:TEAANGLE, 3:+, 4:*, 5:DIAMOND, 6:ARROW, 11:* 14:STAR.

RUN  ARRAY OF RUN NUMBERS.
NDECKS  NUMBER OF POINTS IN RUN.

NOTE: NDECKS IS LESS THAN OR EQUAL TO ZERO, RUN AND IDENT WILL NOT BE DRAWN. THEY MUST still BE SPECIFIED, HOWEVER, IN THE SUBROUTINE CALL.

IDENT  LABEL.

NOTE: IDENT AND JDENT ARE READ IN AS LITERAL DATA, ENCLORED IN PARENTHESES.

NOTE: MICHAJ = -MICHAJ THE FIRST TIME TO CAUSE THE Axis TO BE LABELED ON THE OUTSIDE. MICHAJ = -MICHAJ THE SECOND TIME TO AVOID HAVING THE INTEGER CONSTANT (IE 16) USED AT MICHAJ IN THE CALL TO IMPLOT REDefined AS MISUS THAT INTERE. THIS IS A FEATURE OF FORTRAN.

REAL IDENT, JDENT
DIMENSION IDENT(15), JDENT(15), YLABEL(15), XLABEL(15)

DIMENSION YDATA(MP), XDATA(HP)
CALL PLOT(0., 0., 1.)
HEIGHT-XAXIS -0.1, DISTANCE
CALL PLOTBD(-1, RIGHT, -0.5, 10., 0)

CALL PLOTBD(-1, RIGHT, -0.5, 10., 0)

102 IF NDECKS 106, 100, 102
104 DO 5 K = 1, NDECKS
CALL NUMBER(-0.75, YMIN, 0.14, RUN(K), 90., 0.2)
5 CONTINUE

CALL SYMBOL(-0.75, 6.0, 0.14, IDENT, 90., 0.60)
GO TO 101

106 CONTINUE

CALL SYMBOL(-0.75, 6.0, 0.14, JDENT, 90., 0.1)
101 CONTINUE

IF (NDENOS), 1, 1, 2
2 TNU=0.
DO 6 K=1,NDENS.
   CALL NUMBER (-0.50,TNU,0.14,RUD(K),90.0,2)
   TNU=TNU+0.8
6 CONTINUE
   CALL SYMBOL (-0.50,6.0,0.14,JDENT,90.0,60)
1 CONTINUE
   MICHAR=-MICHAR
   CALL AXIS (0.,0.,YLABEL,MICHAR,10.,90.,THIN,DELY,1.0)
   CALL AXIS (0.,0.,XLABEL,MICHAR,XAXIS,0.,XMIN,DELY,1.0)
   CALL AXIS (XAXIS,0.,-3.,XAXIS,0.,XMIN,DELY,1.0)
   CALL LINE (XDATA,XMIN,DELY,YDATA,XMIN,DELY,SP,JLN,LSY)
   MICHAR=-MICHAR
   CALL PLOTE2
   RETURN
END
2 TNU=0.
   DO 6 K=1,NDEBOS
      CALL NUMBER (-0.50,TNU,0.14,RQD(K),90.0,2)
      TNU=TNU+1.2
   CONTINUE
6 CONTINUE
   CALL SYMBOL (-0.50,6.0,0.14,JDINT,90.0,60)
   CONTINUE
   CALL AXIS (Y,0.,YLABEL,MYCHAR,10.,90.,YMIN,DELY,1.0)
   CALL AXIS (X,0.,XLABEL,MXCHAR,11.,XMIN,DELY,1.0)
   CALL AXIS (XAXIS,0.,-10.0,XMAX,DELY,1.0)
   CALL LINE (XDATA,MIN,DELux,YDATA,MIN,DELY,MP,JLN,LST)
   MXCHAR--MXCHAR
   MYCHAR--MYCHAR
RETURN
END
SUBROUTINE DPLOT(YDATA, XMIN, DELY, YDATA, XMIN, DELX, IAXIS, MP, 
* XLABEL, XCHAR, XLABEL, XCHAR, JLM, LSJ, 
* RON, NDECKS, IDENT, RUD, NDENOS, JDENT)

C
C THIS SUBPROGRAM PLOTS ARRAY YDATA VERSUS ARRAY XDATA IN A STANDARD
C FORMAT. SUBPROGRAM IS DESIGNED TO WORK WITH THE VERSATEC PLOTTER.
C PAGE SIZE IS 8.5 BY 11 INCHES.
C
C PARAMETERS
C
C YDATA ARRAY FOR Y AXIS.
C XMIN VALUE WHICH CORRESPONDS TO THE BOTTOM OF THE PLOT.
C DELY INCREMENT WHICH CORRESPONDS TO ONE INCH OF VERTICAL
C DISTANCE.
C NOTE: Y AXIS IS ALWAYS FOUR INCHES HIGH.
C
C XDATA ARRAY FOR X AXIS.
C XMIN VALUE WHICH CORRESPONDS TO THE LEFT EDGE OF THE
C PLOT.
C DELX INCREMENT WHICH CORRESPONDS TO ONE INCH OF
C VERTICAL DISTANCE.
C XAXIS LENGTH OF X-AXIS. IN INCHES.
C MP NUMBER OF POINTS IN ARRAYS XDATA AND YDATA.
C XLABEL LABEL OF X AXIS.
C XCHAR NUMBER OF CHARACTERS IN THE X LABEL.
C JLM NUMBER OF CHARACTERS IN THE Y LABEL.
C JLN DETERMINES IF DATA POINTS ARE SHOWN OR CONNECTED BY
C LINE SEGMENTS. = 0: LINE SEGMENTS; NO POINTS. 
C = 1: SYMBOL DRAWN WITH LINE.
C =-1: SYMBOL ONLY DRAWN.
C LSJ SPECIFIES THE SYMBOL.
C USEFUL SYMBOLS: 0:BOX, 1:OCTAGON 2:TRIANGLE, 3:+,
C 4:* 5:DIAMOND, 6:ARROW, 11:* 1W:STAR.
C
C RON ARRAY OF RUN NUMBERS.
C NDECKS NUMBER OF POINTS IN RON.
C IF NDECKS IS LESS THAN OR EQUAL TO ZERO, RUN AND
C IDENT WILL NOT BE DRAWN. THEY MUST STILL BE
C SPECIFIED, HOWEVER IN THE SUBROUTINE CALL.
C
C IDENT LABEL
C RUD ARRAY OF RUN NUMBERS, USUALLY FOR DENOMINATORS
C NDENOS NUMBER OF POINTS IN RUD.
C IF NDENOS IS LESS THAN OR EQUAL TO ZERO, RUD AND
C IDENT WILL NOT BE DRAWN. THEY MUST STILL BE
C SPECIFIED, HOWEVER IN THE SUBROUTINE CALL.
C
C JDENT LABEL FOR BACKGROUND.

NOTE: YLABEL AND XLABEL ARE READ IN AS LITERAL DATA, ENCLOSED IN
PARAMETERS.

NOTE: XCHAR= -XCHAR THE FIRST TIME TO CAUSE THE AXES TO BE LABELED
ON THE OUTSIDE. XCHAR= -XCHAR THE SECOND TIME TO AVOID
HAVING THE INTEGER CONSTANT (IE 16) USED AT XCHAR IN THE
CALL TO IRPLOT REDEFINED AS RUDS THAT INTEGER. THIS IS A
FEATURE OF FORTRAN.

REAL IDENT, JDENT
DIMENSION IDENT(15), JDENT(15), XLABEL(15), XLABEL(15), 
* RON(NDECKS), RUD(NDENOS)
CALL PLOT(0.0, 0.1)
RIGHT = XAXIS + 0.1
CALL PLOTBD(-0.5, RIGHT, -0.5, 10.0, 0)
IF(NDECKS) 106, 104, 102
102 TY) = 0.00
GO TO 101
101 CONLOUDE
CALL SYMBOL(-0.75, 0.0, 0.2)
102 CONTINUE
104 CONTINUE
106 CONTINUE
IF(NDENOS) 1, 2
2 YNU=0.
   DD 6 K=1,NDENOS
   CALL NUMBER (-0.50,YNU,0.14,RUD(K),90.0,2)
   YNU=YNU+1.2
6 CONTINUE
   CALL SYMBOL (-0.50,6.0,0.14,JDEMT,90.0,60)
1 CONTINUE
   MICCHAR=MICCHAR
   CALL AXIS (0.,0.,YLABL,MICCHAR,4.,90.,YMIN,DELY,0.8)
   CALL AXIS (0.,0.,YLABL,MICCHAR,XAXIS,0.,XMIN,DELX,1.0)
   CALL AXIS (0.,4.,YLABL,MICCHAR,XAXIS,0.,XMIN,DELX,1.0)
   CALL LINE (XDATA,XHIN,DELX,YDATA,TBIN,DELY,HP,JLN,LST)
   MICCHAR=MICCHAR
RETURN
END
SUBROUTINE SCPLT (YDATA, YMIN, DELT, IDATA, XMIN, DELX, XAXIS, MP, *YLABEL, XCHAR, ILABEL, XCHAR, JLY, LDL, L5Y, *RUN, NDECKS, IDENT, RUD, NDENOS, JDENT)

C**********************************************************
C THIS SUBPROGRAM PLOTS ARRAY YDATA VERSUS ARRAY IDATA IN A STANDARD
C FORMAT. SUBPROGRAM IS DESIGNED TO WORK WITH THE VERSATEC PLOTTER.
C PAGE SIZE IS 8.5 BY 11 INCHES.
C PARAMETERS
C IDATA ARRAY FOR Y AXIS.
C YMIN VALUE WHICH CORRESPONDS TO THE BOTTOM OF THE PLOT.
C DELT INCREMENT WHICH CORRESPONDS TO ONE INCH OF VERTICAL
C DISTANCE
C NOTE: Y AXIS IS ALWAYS TEN INCHES HIGH.
C IDATA ARRAY FOR X AXIS.
C XMIN VALUE WHICH CORRESPONDS TO THE LEFT EDGE OF THE
C PLOT.
C DELT INCREMENT WHICH CORRESPONDS TO ONE INCH OF
C HORIZONTAL DISTANCE.
C XAXIS LENGTH OF X-AXIS, IN INCHES.
C HP NUMBER OF POINTS IN ARRAYS IDATA AND YDATA.
C YLABEL LABEL OF Y AXIS.
C ILABEL LABEL OF X AXIS.
C XCHAR NUMBER OF CHARACTERS IN THE LABEL.
C XCHAR NUMBER OF CHARACTERS IN THE LABEL.
C JLY DETERMINES IF DATA POINTS ARE SHOWN OR CONNECTED BY
C LINE SEGMENTS. = 0: LINE SEGMENTS. NO POINTS.
C = 1: SYMBOL DRAWN WITH LINE.
C >-1: SYMBOL ONLY DRAWN.
C L5Y SPECIFIES THE SYMBOL.
C USEFUL SYMBOLS: 0: BOX, 1: OCTAGON, 2: TRIANGLE, 3: +,
C 4: X, 5: DIAMOND, 6: ARROW, 11: * 14: STAR.
C RUN ARRAY OF RUN NUMBERS.
C NDECKS NUMBER OF POINTS IN RUN.
C IF NDECKS IS LESS THAN OR EQUAL TO ZERO, RUN AND
C IDENT WILL NOT BE DRAWN. THEY MUST STILL BE
C SPECIFIED, HOWEVER IN THE SUBROUTINE CALL.
C IDENT LABEL
C RUD ARRAY OF RUN NUMBERS, USUALLY FOR DENOMINATORS
C NDENOS NUMBER OF POINTS IN RUD.
C IF NDENOS IS LESS THAN OR EQUAL TO ZERO, RUD AND
C IDENT WILL NOT BE DRAWN. THEY MUST STILL BE
C SPECIFIED, HOWEVER IN THE SUBROUTINE CALL.
C JDENT LABEL FOR BACKGROUND.
C NOTE: YLABEL AND XLABEL ARE READ IN AS LITERAL DATA, ENCLOSED IN
C PARENTHESES. PARENTHESES.
C NOTE: XCHAR= MICHAEL THE FIRST TIME TO CAUSE THE AXIIS TO BE LABELED
C ON THE OUTSIDE, MICHAEL THE SECOND TIME TO AVOID
C HAVING THE INTERCEP CONSTANT (IE 16) USED AT XCHAR IN THE
C CALL TO ITRPLOT REDEFINED AS MINUS THAT INTEGER. THIS IS A
C FEATURE OF FORTRAN.
C**********************************************************

REAL IDENT, JDENT
DIMENSION IDENT(15), JDENT(15), YLABEL(15), XLABEL(15),
*RUN(NDECKS), RUD(NDENOS)
DIMENSION YDATA(MP), IDATA(MP)
CALL PLOT(0., 0., 1)
BRIGHT = -1., RIGHT = -0.5, 10., 0)
IF (NDECKS) 106, 103

102
YNU=0.
DO 5 K=1,NDECKS
CALL NUMBER (-0.75, YNU, 0.14, RUN(K), 90.0, 2)
YNU=YNU+0.
5 CONTINUE
CALL SYMBO (0.75, 6.0, 0.14, IDENT, 90.0, 60)
GO TO 101

106 CONTINUE
CALL SYMBO (-0.75, 6.0, 0.14, *90.0, 1)
CONTINUE
IF (NDENOS) 1, 1.2
2 YNU=0
DO 6 K=1,NDEнос
   CALL NUMBER (-0.50,YNU,0.14,NUD(K),90.0,2)
   YNU=YNU+1.2
6 CONTINUE
   CALL SYMBOL (-0.50,6.0,0.14,JDENT,90.0,60)
CONTINUE
   NICHAR'-NXCHAR
   CALL AXSN
   CALL AXIS
   CALL AXIS
   CALL LIHE
   WXCHAR*-NXCHAR
   END
LIST OF REFERENCES


10. O.F. Mossott, Memorie di Matematica e di Fisica della Societa Italiana delle Scienze Residente in Modena, 24, pt 2, 49 (1850).

11. J.C.M. Garnet, Phil. 385 (1904); A205, 237 (1906).


54. Russell, Infrared Absorption of Small Metallic Particles (thesis), The Ohio State University.


