MODELING OF MOLECULAR HEALING FOR MICRO-LASER WELDING OF PLASTICS WITH DIFRACTIVE OPTICAL ELEMENTS AS SPATIAL MODULATORS

A Thesis
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ABSTRACT

This work demonstrated, developed and characterized a new and novel technique for plastics welding using diffractive optics. Using diffractive elements laser beams were reshaped into various geometries that could be used for simultaneous welding of plastic in through transmission infrared welding. This novel technique also included the use of standard optics for resizing diffractive images for microwelding of complex geometries. In addition, new molecular healing models that accurately predict weld size and quality (degree of healing) were developed. The ability to quickly and economically form microwelds is critical to the development and commercialization of polymer-based MEMS and micro-fluidic devices.

Thermoplastics offer significant advantages in the fields of biomedical engineering, communications, and in particular applications related to Micro Electro Mechanical Systems (MEMS). For example, the low manufacturing costs of polymers may allow industry to fabricate disposable MEMS. Rapid, consistent, and inexpensive assembly or packaging is critical to the commercialization of polymer-based MEMS. One method of joining that offers great promise of success for MEMS devices is Through Transmission Infrared (TTIr) welding. TTIr works by passing a laser through one of the components to be joined and focusing it on the second, which has an absorbing material (such as carbon
black) added to it. In the following studies, diffractive optics were used to reshape a laser beam into complex shapes for TTIR welding of plastics. These complex image shapes were then resized to micron-scale for micro-welding of plastics. In this portion of the study, the major findings included but are not limited to the following:

1. The diffractive optical elements could withstand as much as 80 W of laser power
2. The efficiencies of the diffractive optics was greater than 55%
3. Micro-weld features as small as 300 μm with weld lines as thin as 75 μm could be produced
4. Cycle times as short as 50 ms are possible with TTIR welding with beam shaping diffractive optics
5. It is possible to produce hermetic welds that can sustain 0.7 MPa of burst pressure, which based on the weld geometry, results in an average weld stress of 16 MPa and near full parent strength near the edge of the weld.

Another task of this work was to gain a better understanding of molecular healing so that micro-welds could be better understood. Because minimum weld size is affected by competing driving forces, namely thermal conductivity and molecular diffusion, these forces were studied. For example, as time increases heat conduction results in an increase in weld size, thus minimum heating time is desired to produce small welds. In contrast, molecular healing is also proportional to time, thus increasing the heating time increases weld strength. In addition, these two mechanisms are limited by maximum
allowable temperatures, where the base material can degrade or ablate. Thus, increasing the temperatures (power) is also limited.

In this study, it was found that the activation energy for molecular diffusion is temperature dependent. In addition, it was found that by considering the temperature cycle of a weld cycle, better models for predicting the degree of healing can be produced compared to traditional models that rely on a single peak temperature. This model was then coupled with a heat flow model to describe the theoretical limit of micro-welding of plastics. Because thermal diffusion drives a heat source to diffuse outward and because molecular healing is temperature- and time-dependent, there is a limit as to how small a weld can be made. A relationship between the size of a weld and the material properties for a point heat source with different power levels was developed.
Dedicated to the ones I love
Christine, Dad, Mom, Heath and Gianna
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22. David Grewell, Weldability of ABS and Testing of Weld Strength at Various Strain Rates; A Study in Ultrasonic Welding, 55th Annual Technical Conference
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AWARDS

1. Phi Kappa Phi OSU Honors Society, 2003, Baton Rouge, LA


5. Distance mode control for laser welding, US Patent 6,329,629
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LIST OF SYMBOLS

β Angle for spherical coordinates (rad)

δ Position factor

ζ Angle of rotation (rad)

Θ Half angle of ray of light (rad)

θ Temperature (°C)

κ Thermal diffusivity (m²/s)

λ Thermal conductivity (W/(m·°C))

μ Viscosity (poise)

ρ Density (kg/m³)

ϕ Angle for spherical coordinates (rad)

ψ Lens shape factor

ω Optical, angular frequency (Rad/s).

A₀ Diffusion material constant (J)

B Body force (m/s²)

C Specific heat (Joules/(kg·°C))

Dₙ Curvilinear reptation diffusion constant (cm²/s)

Dₜ degree of healing (% or unitless)
E\text{a} Activation energy (J)

f_s Spatial frequency (cycles/m)

h Plate gap height (m)

K Lens geometry factor

k_a Diffusion temperature parameter (1/K)

k Number of iterative try

m Diffraction order

n Index of refraction

P Power (W)

Pr Pressure (MPa)

p Random number

q Heat flux (W/m\(^2\))

Q Internal heat generation (W/m\(^3\))

R Boltzmann constant (J/K)

r Radial flow distance (m)

r_1 Front face radius of curvature (m)

r_2 Rear face radius of curvature (m)

S_2 Distance from the lens to the imaging plane (m)

S_s Ray length (m)

T Absolute temperature (K)

W_0 Minimum spot diameter (m)

n Index of refraction

v Weld velocity (m/s)
u Flow velocity (m/s)

w Heat flow, distance from heat source in x-direction (m)
CHAPTER 1

INTRODUCTION

1.1 POLYMER BASED MICRO-ELECTRICAL-MECHANICAL SYSTEMS (MEMS) AND MICROFLUIDIC DEVICES

With the latest advancements in lithography, microinjection molding, and related technologies it is now possible to manufacture polymer components and machines in the range of microns [1]. For example, it is possible to produce features 10 μm in width by using embossing techniques. In addition, studies in microinjection molding have shown that it is possible to mold complex components, such as gears, with similar dimensions [2].

While there are many interesting applications for MEMS and microfluidic devices, one that is growing very quickly is the use of MEMS in the medical industry. For example, MEMS technology is used to help identify unknown substances or determine key DNA codes from a single drop of fluid. Currently, there are several products on the market that use MEMS technology (see Figure 1.1) [3].
Some of the more complex devices are referred to as “labs-on-a-chip” (see Figure 1.2). These devices have the ability to:

1) **Purify**-Remove any foreign substance from the sample to be studied so that only DNA or other substances of interest remains.

2) **Replicate**-Reproduce the DNA so that measurable amounts are present.

3) **Identify**-Attach DNA to known markers for identification
The use of thermoplastics for these applications offers significant advantages: the low manufacturing cost of polymers allows the creation of low-cost, and ideally disposable devices. In the biomedical industry, the use of disposable devices eliminates the sterilization and cross contamination risks associated with reusable medical devices. This can be instrumental in cost savings, but most importantly it helps to save human lives [1]. The development of low-cost micro-fabrication methods, suitable for high-volume production, is key to the commercialization of polymer micro-system technology [2]. In addition, it has been proposed to replace the silicon chip with chips fabricated from plastics. Other possible applications for plastic-based MEMS are the development of devices that are placed inside the human body. In this case, plastics that are designed to degrade and pass through the body may have significant advantages in aiding the healing process. It should be noted however, that many of these concepts are not yet available commercially, but are under consideration and development at this time.
As can be seen in Figure 1.1 and 1.2, plastics are typically used for the housing and packaging materials of these products. The housing not only protects the silicon-based chip, but it also provides micro-channels that direct the flow of the fluid to different location on the chips (see Figure 1.3). It is important to note that in order to produce micro-channels, two components need to be joined, one component holding the channel and a second component to act as a “lid”. Since the joint must be hermetic, adhesive bonding or welding must be used. Adhesives have the advantage that either no heat or little heat will be introduced into the component. However, adhesives may require significant curing times, they may contaminate the channel or lid above the channel, and they may introduce a source of contamination to a medical device. Welding on the other hand is faster and it requires no new materials at the joint. Therefore, welding the components is the method of choice.

![Figure 1.3 Photograph of typical micro-channels](image)

Figure 1.3 Photograph of typical micro-channels [5]
The assembly of MEMS and the complexity of the minute parts involved require precise control of heat transfer and elimination of vibration that is common in many industrial plastic welding techniques. The minimization of the heat-affected zone and the ability to weld the parts in their final orientation are also important considerations. For example, in order to help promote and control the flow of the fluids through the micro-channels, it maybe necessary to coat the walls and bottom of the channels with chemicals that promote wetting (see Figure 1.4). If the fluids are water-based, such as blood and other bodily fluids, the chemicals will be hydrophilic. In some regions, the coatings can be hydrophobic, acting as valves so that they prevent wetting and flow of the fluid until they are selectively exposed to IR or UV radiation to make them hydrophilic. In most cases, the coating will be temperature-sensitive and will not function properly if over-heated. Thus, it is important to confine any heat generated during welding to the weld zone to prevent damage to the micro-channel. In addition, it will be important to prevent any flash/particulates that are produced during the welding process from entering the channels.
In summary, the joining technique must be able to meet all of the following requirements:

1) Have a small heat-affected zone (HAZ)
2) Not promote product damage by vibrations and relative motion
3) Not produce flash/particulates within the micro-channel
4) Produce strong hermetic seals
5) Have fast cycle times

1.2 CHARACTERISTICS OF PLASTICS

Although polymers in general are often called plastics, there is an important difference. The structure of a polymer is easily deduced from its Greek name: ‘poly’ meaning many and ‘meres’ meaning groups. Thus a polymer is any chemical structure that contains
many repeating small groups linked together to form a structure. Nature forms many polymers, such as cellulose and cotton. In contrast, plastics are man-made polymers. They are very similar to their natural counterparts in that they are formed by many small ‘mers’ (typically carbon-to-carbon functional groups), linked (chemically) together to form a long chain. Compared to natural polymers, such as cellulose, plastics tend to be less environmentally friendly, because they resist chemical break-down. On the other hand, they offer superior properties, such as high thermal stability, which makes them suitable even for “under the hood” components in the automotive industry.

In general terms, plastics are divided into two main categories, thermoplastics and thermosets. The main difference between these plastics is defined by their chemical structures, see Figure 1.5. In thermosets, all chains are connected by primary chemical bonds or cross-links. The cross-links keep the chains well interlocked and provide good thermal and chemical stability. However, the cross-links prevent these materials from being re-formed. Because the thermoset chains are all chemically linked by primary bonds it is not possible to soften them to promote flow by the addition of heat. In contrast, thermoplastics are easily re-formed. The chemical structure of thermoplastics can be imagined as a collection of cooked spaghetti: they are mechanically intertwined and resist relative motion, but their polymer chains are not chemically linked by primary bonds. However, they can deform slowly over time (creep), especially at elevated temperatures. At elevated temperatures, the polymer chains vibrate more vigorously and the average distance between the chains increases, which in turn increases the free volume of the bulk material.
Thermoplastics are comprised of two material categories: amorphous and crystalline thermoplastics. As previously noted, plastics are often modeled as clumps of cooked spaghetti. At a critical average distance, the chain-interaction decreases dramatically and there is a sudden increase in additional free volume. This initial phase change is referred to as the glass transition temperature ($T_g$). Below the glass transition temperature, the plastic becomes glassy and above $T_g$ it will deform significantly under load. If all chains are randomly oriented, the thermoplastic is amorphous. Amorphous thermoplastics tend to soften (decrease in viscosity) gradually with increasing temperature above their glass transition temperature. Semi-crystalline thermoplastics contain regions, in which the chains are tightly packed together in an orderly fashion. These regions are crystalline and do not allow molecular motion to occur until the temperature is above the melt temperature ($T_m$) of the material. In reality, it is difficult to have a fully crystalline polymer with most polymers being semi-crystalline with both amorphous and crystalline regions. The crystalline regions usually have a higher average density compared to the overall average density of the material. Between the $T_g$ of the amorphous regions and $T_m$, these materials will deform slowly behaving like a soft solid. However, above $T_m$, the temperature at which the crystalline regions melt, the bulk material will flow and can be reshaped. Above $T_g$, the plastic is said to become “leathery” and it becomes soft enough to flow [6]. For semi-crystalline polymers, there is a second phase change, $T_m$ (melt temperature), above which the polymer can flow. Thus, thermoplastics can be molded, formed, and welded, while thermosets cannot be re-formed after they are polymerized.
1.3 WELDING OF PLASTICS

Despite the fact that injection molding of thermoplastics can produce complex shapes, joining is still often required to manufacture the final products. For example, to manufacture products with hollow features, two components are usually joined.

In general, there are three techniques that can be used to join plastics:

1) Mechanical
2) Adhesives
3) Welding
Each of these processes has advantages and limitations. For example, mechanical fasteners can be used to join dissimilar materials. However, mechanical fasteners typically do not provide hermetic seals. Thus, the selection of a joining technique must be based on the product requirements. As detailed in Section 1.1, the requirements of many biomedical MEMS dictate welding as the best process to use to assemble these products.

There are a wide range of welding processes used in industry to join plastics. Some of the most common techniques include:

1) Ultrasonic welding  
2) Vibration welding  
3) Heated tool welding  
4) Laser welding  
5) Radio frequency (RF/dielectric) welding  
6) Implant (resistance and induction) welding

It is beyond the scope of this dissertation to detail these processes, but it is important to note that each process has advantages and limitation. For example, the most common process, ultrasonic welding, can weld parts in less than a second, and the capital cost for this equipment is relatively low. However, care must be taken to properly design parts and fixtures to prevent product damage due to the mechanical vibration that are used to generate heat.
Plastics welding processes, while different, have common characteristics. Each technique is comprised of at least five separate steps [7], summarized in Table 1.1. It should be noted that surface preparation is not generally performed for mass production.

<table>
<thead>
<tr>
<th>Step</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surface preparation</td>
<td>• This step can involve cleaning and/or machining of the surfaces</td>
</tr>
<tr>
<td>Heating</td>
<td>• Melt the interfaces to promote flow</td>
</tr>
<tr>
<td></td>
<td>• Heat for this process can be internally generated such as in friction (vibration) welding or externally generated, such as in heated tool welding</td>
</tr>
<tr>
<td>Pressing</td>
<td>• This step involves forcing the molten surfaces together in order to assure they are in intimate contact and promote molecular diffusion and entanglement</td>
</tr>
<tr>
<td></td>
<td>• Force can be applied by an external actuator</td>
</tr>
<tr>
<td></td>
<td>• Force can be generated by thermal expansion of the melt</td>
</tr>
<tr>
<td>Intermolecular diffusion</td>
<td>• The molten surfaces are allowed to stay in contact under pressure for sufficient time to promote molecular diffusion</td>
</tr>
<tr>
<td></td>
<td>• <strong>The time required to allow diffusion is temperature-dependent</strong></td>
</tr>
<tr>
<td>Cooling</td>
<td>• The molten material is allowed to solidify</td>
</tr>
<tr>
<td></td>
<td>• Additional healing (molecular diffusion) can occur</td>
</tr>
</tbody>
</table>

Table 1.1 Detailed description of the separate steps during welding

A detailed description of each of these steps is beyond the scope of this dissertation, but it should be understood that each step is complex and affected by many parameters, such as time, temperature, pressure, and material properties.
One application of laser welding that offers great promise of success is Through Transmission Infrared Welding (TTIr). It works by passing IR radiation through one of the parts while the radiation is absorbed by the other part at their interface. This causes the melting of the base part, which in turn, due to direct contact, results in melting of the transmitting part and the formation of a weld bead at the part interface [7]. Section 1.4.2 provides a detailed description of TTTIr.

1.4 LASER WELDING

There are two basic modes of IR or laser welding [7,8]:

- Surface heating
- Through Transmission Infrared (TTIr) welding

Each will be reviewed separately in the following sections.

1.4.1 SURFACE HEATING LASER WELDING

This technique is very similar to heated tool (plate) welding as shown in Figure 1.6. The surfaces of the components to be joined are heated by direct IR/laser exposure for a sufficient length of time to produce a molten layer, usually for 2-10 s. Once the surface is fully melted, the IR/laser tool is withdrawn from between the parts, the parts are forged together, and the melt is allowed to solidify.
Figure 1.6 Basic steps in the IR/laser surface heating mode of welding

There are two methods of introducing surface heating, scanning (high speed) and continuous illumination [8]. The heating source for continuous illumination with surface heating relies on illuminating the entire faying surface with an array of laser/IR sources. Because surface heating relies on residual heat and melting at the faying surfaces, slow speed scanning is not possible. Instead, only high speed scanning can be used to build up a sufficient melt layer. In this case, the beam is often split with a mirror to illuminate both parts simultaneously, as seen in Figure 1.7. The rotating mirror usually dithers back and forth to direct the beam from one secondary mirror to the other. In addition, it is possible to rotate the secondary mirrors to increase the width of the heated area.
1.4.2 THROUGH-TRANSMISSION IR WELDING

Another mode of IR/laser welding is based on the concept of passing IR/laser radiation (typically with wavelengths ($\lambda$) between 800 to 1050 nm) through one of the components to be welded, while having the second component absorb the light at the interface (see Figure 1.8). This absorption results in heating and melting of the interfaces and allows the parts to be welded.

TTIr welding is used for such applications as automotive lamps and medical components. It is well suited for applications that require hermetic seals with minimal marking and low flash/particulate generation.
The TTIR mode of IR welding is currently the most popular mode of operation, because it offers several additional benefits compared to surface heating. For example, it is a pre-assembled method. This means that the parts are placed into the machine in the same position and orientation as the final assembled position. For many applications, this is critical to allow sub-components to be held in place during the welding process without complex fixtures [9].

Other benefits of TTIR welding include speed and flexibility. A typical cycle time ranges between 1 and 5 s. In comparison, hot plate welding has a typical cycle time of 10 to 30 s. The process can also weld unsupported internal walls with complex curvature if the optical properties allow illumination of the faying surface by the IR/laser radiation. Applications with this type of geometry can be difficult to weld with vibration welding, a process that is considered relatively fast with cycle times of less than 10 s.
Possibly one of the most important advantages of the TTIR process is weld quality. Because the process is non-invasive, the parts typically have excellent cosmetic properties. In addition, there are no excitation vibrations or large heated platens and only the weld area is heated and modified/melted.

One limitation of TTIR is material suitability. One of the components must be relatively transparent to IR radiation. Since most systems on the market use a wavelength between 800 and 1,060 nm, most unfilled polymers tend to be transparent. However, crystalline polymers such as PE and PP tend to promote internal scattering of the radiation. This often limits the clear part to a thickness of less than 3 to 5 mm with scattering materials.

While light and IR radiation generally follows a straight path through plastics, the structure of semi-crystalline materials, such as Nylon (Polyamide PA), polyethylene (PE), and polypropylene (PP), causes internal refraction and scattering, see Figure 1.9. Each phase, crystalline and amorphous, has a different index of refraction and thus the laser light is refracted as it travels through the sample. In the case of a semi-crystalline thermoplastic, a beam will encounter an almost endless number of internal interfaces between the crystalline and amorphous regions within a sample.
This internal scattering only affects a material’s weldability when TTIr is used. The scattering causes the laser light to diffuse as it travels through the sample, reducing the effective energy that reaches the faying surface. If it is assumed that scatter is analogous to absorption, the amount of scatter can be defined by Lambert-Bouger’s Law (Eq. 1.1), in which $I_t$ is the intensity of the light at a thickness (or depth) $t$, through a sample with an absorption constant of $\alpha$ in which the intensity of the applied light is $I_o$. It is important to note that for scatter, $\alpha$ corresponds to the scattering coefficient. Thus, the laser intensity required to melt the interface is proportional to the thickness of the sample when welding diffusive materials, such as crystalline thermoplastics [10,11].

$$I_t = I_o e^{-(\alpha t)}$$  \[1.1\]
In addition the scattering of the light by the crystalline structure effectively increases the travel the light must travel before it reaches the desired weld interface [12]. Thus, further increasing the absorption of the laser energy.

The amount of light that is absorbed by a pure, unfilled thermoplastic is defined by the material’s chemical structure. For example, molecular bonds can be excited to vibrate in particular modes by the absorption of IR radiation. Each mode of vibration is excited by different wavelengths and produces different shapes. While there are many different possible modes of vibration, two common modes are stretching and bending, see Figure 1.10.

![Figure 1.10 Possible modes of bond vibrations: (a) stretching; (b) bending](image)

Historically, the relationship between absorption and chemical structure has been used for material identification. By exposing a sample to a wide bandwidth of IR radiation
(typically a wavelength between 3,000 to 15,000 nm) and observing the absorption, it is possible to determine the type of chemical bonds present, and to interpret a material’s chemical structure [13] (see Table 1.3).

<table>
<thead>
<tr>
<th>Bond</th>
<th>Group</th>
<th>Mode</th>
<th>λ [μm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>C-H</td>
<td>CH₂, CH₃</td>
<td>Stretching</td>
<td>3.3-3.4</td>
</tr>
<tr>
<td>C-H</td>
<td>=C-H</td>
<td>Stretching</td>
<td>3.0</td>
</tr>
<tr>
<td>C-H</td>
<td>-CH₂-</td>
<td>Bending</td>
<td>6.8</td>
</tr>
<tr>
<td>O-C</td>
<td>&gt;C=O</td>
<td>Stretching</td>
<td>5.4-5.9</td>
</tr>
<tr>
<td>O-H</td>
<td>-O-H</td>
<td>Stretching</td>
<td>2.7-2.8</td>
</tr>
</tbody>
</table>

Table 1.2 Selected modes of vibration for some chemical bonds and IR absorption [14]

While the relationship between absorption and molecular structure is advantageous for chemical analysis, it makes most plastics non-transparent to IR wavelengths above approximately 1,600 nm (1.6 μm), except for selected wavelengths that depend on the polymer. As seen in Figure 1.11, common un-filled plastics are relatively transparent from 400 to 1100 nm (0.4 to 1.1 μm). Therefore, wavelengths below 1.1 μm are preferred when welding plastics with TTIr. In addition, the laser light can be easily generated with laser diodes (750 to 950 nm), YAG laser (1060 nm), and quartz halogen lamps (peak intensity at 1100 nm) when welding plastics in a TTIr mode. It is important to remember that most unfilled plastics exhibit this transparency between 400 to 1100 nm, but as previously discussed, semi-crystalline materials encounter internal scatter.
It is also important to keep in mind that not only the physical structure, such as a crystalline structure, of a plastic promotes scattering, but that additives have a similar effect. Additives, such as glass fibers, talc, and inorganic dyes and pigments can promote internal scatter or absorption. Organic dyes tend to dissolve within plastics and usually have a particle size (or molecule) much smaller than the wavelength of light (EMR), and therefore do not promote refraction [16]. That is to say, shorter wavelengths or larger particle size tend to produce more scatter.
In addition to requiring that one part be transparent to the radiation, the other part must be absorbent. Usually, this is accomplished by the addition of carbon black or an IR absorbing dye.

To produce IR radiation, there are two primary sources; IR lamps and IR lasers (such as YAG laser). IR lamps, such as quartz halogen lamps, have the advantages that they are relatively inexpensive and require simple power supplies. However, in order to produce near IR radiation, the tungsten filament must be very hot and thus has a limited life expectancy. While halogen added to the bulb gasses increase the life of the lamp, it is still limited. Another major disadvantage to quartz lamps is that while they produce the maximum intensity at a given wavelength, they also produce a relatively wide distribution of light, as shown in Figure 1.12. In terms of TTIr welding, the longer wavelengths (+1000nm) can be absorbed even by the relatively transparent plastic component and produce undesired heating.
Lasers have the advantage of producing monochromatic radiation, and thus have higher transmission through most plastics. However, compared to quartz halogen lamps, lasers are relatively expensive.

1.4.3 CURRENT TECHNOLOGY OF LASER RADIATION

In TTVr welding, there are several techniques for applying or directing the radiation to the bond line (faying surface): scanning of the weld area by moving either the parts or the laser, simultaneous heating of the joint area, and masking.
1.4.3.1 SCANNING

The scanning technique involves translating an IR/laser source across the faying surface. This approach usually involves locating the parts in a fixture and translating the IR source with a robotic arm or similar type of automation. One of the main advantages of this approach is that a single welding machine can be easily re-programmed to weld a variety of part geometries. However, one limitation of this approach is the fact that the faying surfaces must be in intimate contact. This is because, as the IR source translates around the circumference of the part, the faying surface is only locally heated (see Figure 1.14). Thus, unless the parts are compliant and can be locally deformed to force the faying surfaces together, any gaps between the faying surfaces can result in weld voids. Gaps between the two parts can be the result of molding warpage, molding shrinkage, ejector-pin indentations, or variations in the mold cavities.

Small gaps can be welded or sealed as a result of thermal expansion as the plastic heats and melts. The size of the gaps that can be fully welded or sealed depends on the welding parameters as well as on material properties, such as the coefficient of thermal expansion (CTE) which defines how much a material expands upon heating. Figure 1.13 shows weld strength as a function of defect size for welds made with (AWS G1.2-Standard) [17] samples. It is seen that there is a significant loss in weld strength with defects as small as 0.25 mm [18]. It is important to note that for the scanning welds, the laser beam did not fully cover the width of the web. Therefore, when calculating the weld strength using the web width, the scanning welds appear weaker. The material in this study (Aliphatic
Polyketone) is a highly crystalline material with a relatively high CTE, (25 to 55°C) 1.9x10^-5 cm/cm/°C.

Figure 1.13 Example of weld strength as a function of weld defect for two modes of IR welding (courtesy Branson Ultrasonics Corp.)

Figure 1.14 IR/laser scanning and localized heating
The typical diameter of an independent beam ranges from 0.6 to 2.6 mm which allows the welding of intricate patterns as shown in Figure 1.15.

![Typical weld with scanning](image)

Figure 1.15 Typical weld with scanning (courtesy Leister Corp.)

A basic square, circle, rectangle, or other contour can be sealed with travel speeds ranging from 10 to 50 mm/s. Multiple banks of laser heads are concurrently used, allowing for batch processing and higher production speeds.

When welding a square pattern, or any pattern with sharp turns or bends, the degree of heating of the plastic in the corner or sharp contour areas will be higher. Precise Proportional Integral Differential (P.I.D.) control can be utilized with the single beam method to control or reduce the intensity of the light as the beam passes over the intricate
corners or contours. This will eliminate over-welding in condensed weld areas and ensure an even weld width throughout the weld pattern.

In many instances, especially with micro fluidic or sensing devices, displacement or collapse of the substrates is not tolerable, as it will affect the fluidic channel size or final part height. Inherent in this method is the benefit of a fixed or mechanical stop, providing identical and consistent stack heights before and after the welding process.

1.4.3.2 QUASI SIMULTANEOUS HEATING

An alternative mode of IR scanning uses a light source that is translated around the part at a high velocity so that the beam returns to any given point before the material is allowed to solidify. This allows for the entire faying surface to be melted during the weld cycle. Unless the part is relatively small, the minimum scanning rate requires the beam to be translated with galvanic mirrors or a very fast robotic system. If galvanic mirrors are utilized, the IR source is usually limited to a laser source in order to keep the beam collimated as it reflects off the mirrors. This mode has the advantage that melt-down or collapse for the whole weld area is possible. Thus, virtually any gap size can be welded or sealed with the proper amount of melt-down. It also retains the benefit that a single welding machine can be easily re-programmed to weld a variety of joint geometries. If galvanic mirrors are used however, the application must be relatively planar so that the
beam can be translated around the part without being blocked by the part itself or by appendages. These areas are known as “shadow” areas. That means that the part geometry must allow for the entire faying surface to be illuminated from a single point with the rotating mirrors.

1.4.3.3 SIMULTANEOUS HEATING

The third possible heating mode for TTIr is continuous illumination. In this mode, there are numerous IR sources illuminating the entire faying surface during the weld cycle (see Figure 1.16). As with high-speed scanning, part tolerance and fit-up are not as critical since melt-down is possible. In addition, complex geometries can be welded without the limitation of shadow areas and there are no problems with “run-on/run-off” (where “run-on/run-off” are defined as regions where the weld is started and stopped). These regions represent transition zones and often contain defects because of the transitions.

Figure 1.16 Continuous illumination with IR welding (courtesy Leister Corp.)
If complex geometries are to be welded, it is possible to use a flexible array of diodes, as shown in Figure 1.17 [19]. In this case, a plurality of laser sources are used and mounted on a flexible backbone. The backbone keeps a relative constant distance between the individual diodes and allows electrical connections. The spatial geometry of this backbone is then matched to spatial relationship of the weld geometry.

![Figure 1.17 Continuous illumination with IR welding (courtesy Branson Ultrasonics)](image)

In addition, it is possible to use light guide technology so the laser sources can be remotely located from the work piece for better uniformity and longer product life [20]. In these examples, hybrids of fiber optic cables and 2-dimesional wave guides, such as sheets of polycarbonate or silicone, have been used in order to promote highly uniform welds. That is to say, by randomizing a large number of fiber optic cables (+20,000)
coupled to a small number of sources (19 to 52 sources), any fluctuation in the intensity of any one source is normalized at the target. In addition, by using 2-dimensional light guides (sheets), additional randomization of the light can be achieved in order to ensure uniform heating at the weld zone (target).

1.4.3.4 MASKING

A fourth possible heating mode for TTIr is mask welding. This technique utilizes a typical continuous illumination curtain of light that is passed over a mask blocking portions of the light, allowing only the pre-specified areas to melt and seal. An example of this method is shown in Figure 1.18. This method is especially suited for complex, micro-structured areas. Micro welds as narrow as 100 μm can be achieved (Figure 1.19). The correlation of light intensity, clamping force, and travel speed (the speed of the laser passing over the mask or the mask assembly passing under the laser) controls the amount of melt and edge definition.
As assemblies become smaller and more challenging, the requirement for precise alignment of the mask, the top component, and the bottom component becomes more critical.
1.5 PROPOSED APPLICATION OF LASER RADIATION BY DIFFRACTIVE OPTICS

The novel welding technique that is proposed in this research is the use of diffractive elements (DE’s) for laser beam shaping [21]. That is to say, a collimated laser beam, such as a beam from a YAG laser, can be passed through a specially designed lens that reshapes the beam to match the spatial relationship of the desired weld pattern. The concepts, design, and fabrication of DE’s are detailed in Sections 2.1.1, through 2.1.3, but for the present discussion it will be taken that a hypothetical DE has an optimized design and fabrication. In this case, when a laser beam passes through the DE, the beam is reshaped with a relatively high level of efficiency, above 75% [22]. The beam does not immediately take the proper shape after passing through the lens, but does so after some critical distance proportional to several design parameters, such as DE’s feature size and laser beam wavelength. The pattern then continues to diverge proportionally to these same design parameters. Figure 1.20 shows the proposed welding technique where the desired weld pattern is a simple ring. It is important to note that it is possible to design DE’s that can generate very complex shapes.
Figure 1.20 Proposed use of DE’s for TTlr laser welding of plastics

Some of the advantages of the proposed technique include:

1) Relatively simple optical components,
2) No need for complex light guides [20],
3) Relatively efficient,
4) Ability to illuminate complex shapes.

Some of the limitations of the proposed technique include:

1) Each application requires a special lens design
2) The raw beam must be planer/collimated
3) The image is focused in a 2-dimensional plane.
Currently, the entertainment industry [23] uses computer controlled DE’s, so called spatial modulators, that can be reprogrammed to generate random patterns. This eliminates the need to design and fabricate a new lens for each application. However, the current technology of these devices, prevent them from being useful at relatively high powers (+100 mW) where they can be employed to make welds. However, it is believed that in the near future this limitation will be overcome and lens fabrication for each new part geometry will no longer be required.

Traditional algorithms that are used to design DE’s (Fourier Transforms) rely on the assumption that the raw beam is collimated. As will be detail in Section 2.1.2, this minimizes the computational requirements during the design phase. However, it is theoretically possible to start with a more fundamental assumption, such as the Maxwell Equations and design a lens that can start with any predefined raw beam shape. In this case, the computational requirements are relatively intensive. However, this type of design would allow the use of relatively low-cost laser sources that do not produce raw collimated beams, such as laser diodes (~10 US$/W), to be coupled directly to DE’s. In contrast, the typical cost of a YAG laser is approximately 100 times this cost. The issue with low-cost laser sources (laser diodes) is that they have a relatively high beam divergence and have anisotropic divergence. In addition, in order to produce relatively high powers (+2 W), many individual emitters (19-21) are placed side-by-side. It is common to couple the raw beam with cylindrical lens to reduce the divergence of the “fast-axis” from ~90° to ~3°(see Figure 1.21); however, even with this correction, Fourier transforms cannot be used to design DE’s. It is important to note that these low-
cost devices can be used with DE as long as the beam is well defined and proper assumptions are made in the model to account for the raw beam spatial definition. In addition, the model must start with the fundamental wave equations. Thus, only DE’s designed with simply transformations (Fourier Transforms, detailed in Chapter 2) require a collimated beam from a relatively costly laser.

![Figure 1.21 Laser beam divergence from typical laser bar diode](image)

Another limitation that can be eliminated, is that the beam pattern is restricted to 2 dimensions. By using holographic techniques, it is possible to produce 3-dimensional patterns. It should be noted that it is possible to use computer algorithms to produce holographic images (3-D) but because of the computational efforts, this is not typical. The functionality and fabrication of holograms are detailed in Section 2.1.1 and 2.1.3,
respectively, but it will be stated here that there are several key differences of holograms (a family of diffractive elements) compared to computer generated DE’s. First, because holograms are produced experimentally, there are no approximation errors as commonly seen with computer generated DE’s, thus they are more efficient, as high as 90-95%. That is to say as much as 95% of the laser power going into the lens will be delivered to the target image. This increase in efficiency is primarily the result of no losses due to off orders of diffractions \((0^{th}, 2^{nd}, 3^{rd}, \text{ etc.})\), caused by truncation and other approximation errors in computer generated DE’s. The concept of diffractive order is detailed in Section 2.1.1, but the main point at this time is that holograms are inherently efficient DE’s. Lastly, as noted, holograms can generate 3-dimensional complex patterns, which allow complex geometries to be welded. For example, in welding of an automotive tail-light, the part and weld lines have a 3-dimensional curvature and shape. Thus, the use of holograms to reshape the beam would be ideal. However, one major limitation to holograms is that they require a highly spatially coherent light source, such as those produced with long resonant cavity lasers.

1.6 LITERATURE REVIEW

Becker and Gärtner [1] pointed out that it is important to develop methods for assembling MEMS devices. They proposed the use of ultrasonic and laser welding but left the development of these technologies to other investigators.
Kim and Xu [24] studied the use of continuous wave (CW) laser sources with a wavelength of 1100 nm to weld small-scale plastic components. They were able to demonstrate spot welding with diameters of approximately 400 μm with acrylic samples. In this study, the welding configuration was TTIr. Kim and Xu reported the generation of bubbles when energy levels were too high, 60 s at 0.42 W/mm² (29.1 mW). The generation of bubbles in the weld zone is well understood for other processes. For example, Potente [25] showed that bubbles can be generated in vibration welding if the vapor pressure of the bubble exceeded the weld or clamp pressure, assuming that sufficient time for molecular diffusion of water molecules is allowed. If it is assumed that bubbles can be generated by the same process in laser welding, then it is easy to see that with increased power there is an increase in temperature and vapor pressure promoting porosity (bubbles). However, it is important to note that laser heating can result in very high temperatures that can cause degradation as well as out-gassing resulting in porosity. This process is not fully understood, but the Food and Drug Administration (FDA) [26] defines that polymer degradation can be initiated with power densities as low as 1000 W/cm².

Russek et al., [27] evaluated the welding of PC and acrylic by TTIr on a relatively small scale, a weld spot of approximately 500 μm in diameter. In their study they found porosity in the center of the weld when relatively high heat inputs where used (10-15 J/cm for polycarbonate). The publication did not report the level of heat input required to promote the porosity, but it was theorized that it was caused by over-heating of the polymer and out-gassing. The study did show weld strength as a function of weld gap, or
miss-fit between the weld samples. They found that with scanning, gaps as small as 250 to 500 μm, depending on weld geometry, could prevent welding. In contrast, they also found that continuous illumination was not affected by gap size.

1.7 PROPOSED APPROACH OF MICRO-LASER WELDING

Because a “real” image is produced with diffractive optics [22], it is possible to further manipulate the image with standard optics. For example, by passing the image through a convex lens, it is possible to reduce the size of the image at a given plane, see Figure 1.22. This allows micro-features to be welded. In addition, by placing the lens on an actuator, it is possible to have the lens move relative to the parts to ensure proper welding. This is similar to the technology used in standard CD-music players [28].

Figure 1.22 Diffractive optics coupled with a convex lens for image re-sizing
It is also possible to use one DE and focusing lens to weld an array of geometries. For example, by placing a galvometric mirror between the convex lens and the part, it is possible to steer the image from one location on a part to another. This may prove very useful when welding bio-medical application, where a medical tray may contain as many as 46 to 96 individual identical assays (test sensors). It is important to note that in this configuration, the distance between the mirror and the part must be relatively large, in order to keep the angle of incident constant and assure relatively uniform heating. Thus, by designing the optical components, including the DE, properly, it is possible to have the incident angle for all essays to be heated/welded uniformly. It is also important to note that the laser must be switched on and off between translation from one weld to another and the DE can be designed to weld a multitude of assays simultaneously in order to increase manufacturing capacity.

1.8 DIFFRACTIVE OPTICS AND MOLECULAR HEALING

While the topics of diffractive optics and molecular healing may appear to be unrelated, in this work it will be shown that in order to further develop the technology of micro-welding (welds smaller than 500μm) of plastics, molecular diffusion is critical to understanding micro-welds made with diffractive optics. For example diffractive optics can be used to reshape a laser beam into predefined shapes, such as circles, boxes, crosses or any other shape. In addition, these shapes can then be resized using standard optical components. That is to say, it is possible to resize these images to a very small scale in order to make micro-welds with plastics. While there are optical limitations on the
focusing of an image and the smallest achievable image size, the final limitation that may define the smallest achievable weld can be defined by heat flow (thermal diffusion) and molecular healing (molecular diffusion). Many optical limitations can be overcome with better quality optical components and system design. However, it is proposed that because thermal and molecular diffusion are fundamental processes, minimal weld size will be limited by these factors and not optical designs. Thus, this work will evaluate diffractive optics and focusing of diffractive optical images for micro-welding of plastics and compare the minimal achievable weld size to theoretically predicted weld sizes. These topics and their relationships are shown in Figure 1.23.

Figure 1.23 Overview of proposed research topic
1.9 OBJECTIVES

The objectives of this study were to:

1. Develop a molecular healing model that allows time/temperature histories to be used to accurately predict weld widths.
2. Verify that the molecular healing activation energy is temperature-dependent and determine the relationship between activation energy and temperature.
3. Couple molecular healing models with thermal models.
4. Develop theoretical minimal weld sizes based on molecular healing and thermal models.
5. Demonstrate the use of diffractive optics for beam shaping in laser welding of plastics.
6. Generally determine process parameters for diffractive TTIr welding and weld quality. In particular, determine the general relationships between power and time to weld size and weld strength.
7. Demonstrate the use of image size reduction using standard optics for micro-welding of thermoplastics.
CHAPTER 2
DIFFRACTIVE OPTICS

2.1 DIFFRACTIVE OPTICS

As previously noted, it is possible to use diffractive optics to reshape a laser beam and other light sources into complex shapes. As the name implies, diffractive optics function by diffracting light. Unlike standard optics that bend light through refraction, diffractive lens rely on the superposition of waves. Because these optics function by inference of waves that have defined phase shifts, it is important to gain insight into the details of the functionally, design, fabrication and most of all, how these optical elements can be used to make welds. This chapter covers each of these topics.

2.1.1 FUNCTIONALITY OF DIFFRACTIVE OPTICS

The basic functionality of DE’s is based on wave superposition and destructive and constructive interference. In a very simple example, a collimated beam that passes through two relatively thin slits in a mask, will produce interference patterns on a screen at some distance from the slits [23], see Figure 2.1.
In this simple example, the resulting patterns are well defined and can be easily predicted. For example, using the model of a mask with two slits, it is possible through geometry relationships to show that the distance $y$ between adjacent bright spots (constructive interference) can be determined using Eq. 2.1 [29], where $\lambda$ is the wavelength of the light and $m$ is diffractive order and is any integer. The balance of the variables are detailed in Figure 2.2. It is important to note that for a clear diffractive pattern to be formed, the light source must be well collimated before it strikes the mask. Collimated sources include lasers and very distant spherical sources (light bulb).

$$y = \frac{m\lambda D}{d}$$

[2.1]
A very similar effect as the one illustrated in Figure 2.1 can also be formed by using a transparent window (plate), in which the slits are replaced by local changes in window thickness, see Figure 2.3. In this case, the change in the depth of the local regions causes a change in the path length of the light. Because of the difference in index of refraction of the relative materials, in this case glass and air, the light passing through the thicker regions of the lens is slowed relative to the light passing through the thinner regions of the lens. If the slowing of the light is equal to half the wavelength of the light, the effect is similar to the one detailed in Figure 2.1, except that instead of a significant portion of the light being masked, nearly all of the light is allowed to pass through the lens. This greatly increases the efficiency of the lens, which can be as high as 70%. However, because the lens is designed to slow the light by half a wavelength, it is only fully effective with light from a monochromic source at the proper wavelength. That is to say,
if the lens is used with a wavelength different than its design wavelength, its efficiency will be greatly reduced.

Figure 2.3 Illustration of diffractive pattern from thickness change in window

For reference, DE’s that rely on masking are often called magnitude lenses while DE’s relying on phase shifts are typically called phase diffractive elements.

Further efficiency of the element can be achieved by adding additional depth changes. For example, instead of designing the element with only two levels, it is possible to design it with multiple depth levels, each equal to fractions of the full wavelengths. In this case, it is typical to produce elements with 4 or 8 levels. In the case of a four level element, each level produces a shift in the wavelength as detailed in Table 2.1. The relative phase shifts produce partial destructive and constructive interference regions, which in effect allow better resolution of the desired image compared to a 2 level design.
A similar effect is seen when infinite series of sine functions are used to approximate a square wave.

<table>
<thead>
<tr>
<th>Depth</th>
<th>Fraction of wavelength</th>
<th>Phase Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0°</td>
</tr>
<tr>
<td>2</td>
<td>¼</td>
<td>90°</td>
</tr>
<tr>
<td>3</td>
<td>½</td>
<td>180°</td>
</tr>
<tr>
<td>4</td>
<td>¾</td>
<td>270°</td>
</tr>
</tbody>
</table>

Table 2.1 Detailed phase shifts at various elements depth (0-180 phase change)

### 2.1.2 DESIGN OF DIFFRACTIVE OPTICS

In order to produce 2-dimensional patterns, such as the circle depicted in Figure 2.4, the line mask as previously detailed is replaced by a 2-dimensional pattern, which appears very complicated. For example, Figure 2.5 shows a diffractive pattern which, when illuminated with a uniform collimated beam, produces a circle. In order to design this pattern, Inverse Fast Fourier Transforms (iFFT) of complex arrays are performed [30].

![Figure 2.4 Example of desired pattern produced by diffractive optic](image)
In more detail, in order to design a mask to produce a circle, the image is constructed as a bitmap graphic, based on the intensity mapping of the image. For example, a zero (0) is assigned to black regions of the bit map and a 255 level is assigned to white regions. It is important to note that the absolute values of the assignment of the levels is not critical. For example, a scale from 0 to 10 could also be used. Next, a random phase \((B_{x,y})\) is added to each cell/pixel of the bitmap and the magnitude of the real component (A) is adjusted so that the magnitude of the vector remains the same as the original magnitude \(|f_{x,y}|\), see Eq 2.1 and Figure 2.6 where \(i\) is the square root of -1. The random phase is added in order to account for the real property of light that has a random phase.

\[
|f_{x,y}| = |A_{x,y} + (B_{x,y} \cdot i)| \tag{2.1}
\]

Where \(jx, jy\) are indices of the array. The random phase is adjusted by varying the amplitude of the real and imaginary components of the vector.
Figure 2.6 Details of random phase addition and magnitude retention

The image is then inverted from the center to the corners, see Figure 2.7. This is because a diffractive element acts as both a lens, which inverts an image and a mirror, which flips an image.

Figure 2.7 Example of image inversion with a circle image
Next, an inverse (iFFT) is performed on the inverted image based on Eq 2.2 [31].

\[
F(f_x, f_y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y) e^{-i2\pi(f_x x + f_y y)} \, dx \, dy
\]  \[2.2\]

Where \(f(x, y)\) is the complex value the original values (complex amplitudes) of the bit map. In addition, \(f_x\) and \(f_y\) are the spatial frequencies of the FFT. For example (see Figure 2.8), if a beam light passes through a coordinate system at some angle, then the spatial frequencies, (cycle/m) are dependent on the beam of light and the angle of incident.

![Figure 2.8 Details of axis dependent spatial frequencies](image)

Figure 2.8 Details of axis dependent spatial frequencies
The phase portion of the complex values of the iFFT are then truncated to 2, 4 or 8 levels, depending on the number of levels that will be fabricated in the final element. The efficiency of the final elements is related to the number of levels. In this study, only two-level and four-level elements were designed. In the case of two-level design, the values are truncated to either 0° or 180° phase change; in contrast, in the four-level designs the phases were truncated to 0°, 90°, 180° and 270° phase changes. That is to say, instead of designing the element to block approximately 50% of the light as previously detailed (called a magnitude diffractive optic design), the element will allow approximately 100% of the light to pass through the DE. This is accomplished by using the same design as previously detailed, but slowing down portions of the light instead of blocking portions of the light. That is to say, it is possible to fabricate an element with local thickness changes equal to the fractions of wavelength of light in the element media. Thus, when the light exits the element, the phase difference of the individual elements results in the destructive and constructive interference, see Figure 2.3. With this type of element and with the proper design, it is possible to achieve greater than 70% efficiencies.

In order to determine whether the proper image will result from the predicted mask, a forward FFT can be performed on the mask array using Eq 2.3 [31].

\[
f(x, y) = \frac{1}{(2\pi)^2} \int \int F(f_x, f_y) e^{i2\pi(f_x x + f_y y)} df_x df_y \tag{2.3}
\]

As seen above, the magnitude is reduced by a factor of \(1/(2\pi)^2\) compared to iFFT, therefore the magnitude has to be adjusted accordingly. Also, the image must again be inverted from
corners to centers. This is because the Fourier transforms do not include the physical aspect of ray tracing that occurs when the actual element is illuminated to produce an image.

This methodology of DE design is referred to as a direct design, which typically results in non-optimized performance and has many possible solutions depending on the values of the random of the phase that are used (Eq 2.1). Thus, the direct method will most likely not produce the most efficient design. For example, a significant amount of energy of the original beam will be passed through the zero order, which corresponds to passing straight through the center, as seen in Figure 2.9. This “hot-spot” can be masked out with a spatial filter as shown in Figure 1.22. Other artifacts of a direct design include, 2\textsuperscript{nd}, 3\textsuperscript{rd}, etc. orders being formed, which further reduces the efficiency of the element as well as producing noise within the image that makes it fuzzy (low fidelity), see Figure 2.9.
In order to improve the design of a DE, alternative techniques (encoding), based on stochastic algorithms, have been developed which produce much higher efficiency DE’s compared to the DE’s designed with the direct technique. That is to say, they have lower intensity $0^{th}$ and $2^{nd}$, $3^{rd}$, etc., order diffractive images and most of the energy is delivered to the desired $1^{st}$ order image. There are a number of methods (often called bidirectional algorithms) used to find an optimum design for diffractive optics, including but not limited to:

- Genetic coding algorithms
- Annealing
In general, these techniques randomly apply changes to a randomly generated solution in order to find a better alternative solution. In more detail, the predicted pattern from the randomly generated DE ($f^2(x,y)$ as seen in Eq 2.1) is compared to the desired pattern ($f^1(x,y)$) using a merit function (Eq 2.4). The DE is then randomly altered slightly and a new merit function is calculated in order to determine if the alteration improved the DE design. This is repeated until a reasonable desired pattern is produced [32]. This type of approach is typically computationally intensive.

$$Merit = \frac{1}{jx, jy} \sum_{jx, jy} (|f^2(x, y)| - f^1(x, y))^2$$

[2.4]

One of the less computationally intensive methods is annealing (simulating annealing). While annealing is relatively fast, it can produce DE’s with efficiencies as high as 85%. The basic premise of annealing is that in addition to the standard variables found with DE design, namely phase for a given array index, there is an additional variable, p. This variable p is also randomly selected during each iterative try (new random change of mask). During each iteration try, if a randomly selected change to the DE’s improves its performance, it is not automatically accepted. Instead, p is compared to the reciprocal of the iterative try, k. If p is less than k, and the change decreases the merit function (better design) and only then the change is accepted. For example, if at the 100th try (k=100), a better DE pattern is found, this better design is only accepted if $p < 1/100$. Thus, as the
number of iterations increases, the probability of accepting a change decreases \((1/k => 0)\).

See Figure 2.10 for more details.

This type of stochastic approach is often compared to the annealing of metals. For example, by increasing the initial value of \(k_0\), it is possible to increase the probability of accepting a change. Thus, initially changes are accepted quickly. This is similar to fast cooling of a melt where numerous, small grains are formed. In contrast, if the cooling is slow, analogous to a low \(k_0\) value, the changes are not quickly accepted and in the case of metal, the grains are less numerous and large. Thus, better DE’s designs are typically found by only accepting limited changes and making fewer changes as the stochastic process proceeds.
2.1.3 FABRICATION OF DIFRACTIVE OPTICS

As noted in Section 2.1.1 and in particular in Eq. 2.1, \( y = \frac{m\lambda D}{d} \) the divergence of an image \( y \) is inversely proportional to the pitch (distance between diffractive pixels \( d \)) and proportional wavelength \( \lambda \). Because the wavelength of light is relatively small (400 to 700 nm) and even with a YAG laser, the wavelength is still only 1084 nm, the pitch of most DE’s are between 5 and 25 \( \mu \text{m} \). In detail, the pixels of a DE must have widths and heights between 5 and 25 \( \mu \text{m} \). If the pitch is significantly greater than 25 \( \mu \text{m} \), the working distance (distance between DE and image plane/weld) becomes large and often impractical. Thus, methods to fabricate a element with feature sizes in these ranges include:

- **Micro-machining** [33] where very small bits (<20 \( \mu \text{m} \) in diameter) are spun at very high angular velocities (>100,000 rpm)
- **Direct writing methods** [34], where electron beam or laser energy is focused to a very small spot (<10 \( \mu \text{m} \) and material is removed by ablation and a pattern is generated using a rastering technique.
- **Lithography techniques**, where a mask that is generated with direct writing techniques is used to image a desired pattern on a substrate with photo-chemical exposure.
While there are other techniques or variations of these techniques, such as hot embossing or laser assisted embossing [35], it is common to use some variation of lithography. The main reason is that direct writing methods require long machining times because of the amount of material that must be removed, and micro-machining often results in non-optically smooth surface, in addition, square patterns of the desire sizes are difficult to achieve. Accordingly, in this work only lithography will be described as a fabrication technique for DE elements.

The basic concept of lithography relies on having a mask with an image of the desired features. Typically, this mask is fabricated with a chrome-coated glass plate that is either laser- or EB-patterned. This image is then transferred to a substrate coated with a light-sensitive chemical so that either a negative or positive image of the original remains. An etching method is then used to remove material from the substrate. After a predetermined amount of material is removed, the remaining photoresist is removed.

There are six major steps involved in lithography:

1) Substrate preparation, usually involving cleaning and surface modifications for adhesion.
2) Spin coating of a photosensitive chemical (photoresist) on the surface of the substrate.
3) Alignment of the mask to the substrate.
4) Exposure of substrate and mask to light (typically ultra-violet light)
5) Development of the photoresist.

6) Etching of the substrate.

2.1.4 LITERATURE REVIEW FOR DIFRACTIVE OPTICS

In terms of using diffractive optics for high power applications, there are limited references. Liu (et al. [36]) used diffractive optics for beam shaping as a launching mechanism into fiber optic cables. That is to say, they fanned out a single beam into various numbers of beams (2, 4, 8 and 10) in order to couple the original single beam to fiber optic cables. They also reshaped circular beams into rectangular top hat beams for material processing. They based most of their diffractive patterns on improved annealing algorithms and were able to achieve efficiencies as high as 85% with 16 level diffractive orders. One of the reasons they were able to report such high efficiencies was that they not only designed images that were in the 1st order, but also designed the function of the element to make use of the higher order patterns. Thus, they used the higher diffractive patterns. This effectively reduced losses in the higher orders. They did not implement their design into any application and worked with a YAG laser with powers greater than 100 mW. Kawamoto [37] proposes using diffractive optics for welding of plastics using a YAG laser. The proposed welding configuration is similar to those proposed in this research; however, there was no details provided, such as diffractive design algorithm, power levels, efficiencies and fidelity by Kawamoto at this time.
It has been reported that diffractive optics can be used to drill composite substrates for the electronic industry [38]. In this case, a single beam from a YAG laser is reshaped to match the desired hole pattern. In addition, Lizotte reported that diffractive optics can be used to weld High Intensity Discharge (HID) lamps for the automotive market. In this case, a laser beam is reshaped to match the circle pattern to braze the diameter of the lamp [39].

2.2 EXPERIMENTAL PROCEDURES WITH DIFFRACTIVE OPTICS

2.2.1 MATERIALS AND SAMPLES

Two thermoplastic materials were used in this study, polycarbonate (PC) and polystyrene (PS). They were selected because they represent materials that will probably be used in the MEMS industry. Tables 2.1 and 2.2 provide details of mechanical and thermal properties for these materials.
<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trade name</td>
<td>Hyzod</td>
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<tr>
<td>Density</td>
<td>1202 Kg/m$^3$</td>
</tr>
<tr>
<td>Tensile strength yield</td>
<td>62.05 MPa</td>
</tr>
<tr>
<td>Tensile strength ultimate</td>
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</tr>
<tr>
<td>Tensile modulus</td>
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<tr>
<td>Thermal conductivity</td>
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<tr>
<td>Specific heat</td>
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</tr>
<tr>
<td>Tg</td>
<td>150 °C</td>
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<tr>
<td>Carbon black</td>
<td>0 and 0.1%</td>
</tr>
<tr>
<td>Clear sample thickness</td>
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</tr>
</tbody>
</table>

Table 2.1 Mechanical and thermal properties of polycarbonate[40]

<table>
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<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
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<tr>
<td>Density</td>
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<tr>
<td>Tensile strength yield</td>
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<td>Tensile strength ultimate</td>
<td>25.02 MPa</td>
</tr>
<tr>
<td>Tensile modulus</td>
<td>1,862 PMA</td>
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<tr>
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<tr>
<td>Specific heat</td>
<td>1423 J/Kg°C</td>
</tr>
<tr>
<td>Tg</td>
<td>80 °C</td>
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<tr>
<td>Carbon black</td>
<td>0 and 0.6%</td>
</tr>
<tr>
<td>Clear sample thickness</td>
<td>0.25 mm</td>
</tr>
</tbody>
</table>

Table 2.2 Mechanical and thermal properties of polystyrene [41]

Two main images were used to characterize welds made with diffractive optics, a circle and a square, as shown in Figure 2.11. The size of the welds (diameter and width
respectively) was determined by the distance between the diffractive optic and sample (working distance). The widths of the weld lines were determined by varying the process parameters, namely laser power and weld time.

Figure 2.11 Details of weld samples for diffractive optics

2.2.2 DIFFRACTIVE OPTIC DESIGN AND FABRICATION

Two diffractive optical designs were studied:

1) Direct method

2) Annealing method

For direct algorithms, a MathCad file was used to predict the desired diffractive patterns (see appendix). In this case, the desired image was a 50 x 50 two level (0 and 255) bit map. Thus, the resulting diffractive image was also a 50 x 50 image. Depending on the
final feature size (size of each pixel), the diffractive image was tiled repetitively so that the entire beam (3 mm in diameter) was captured. That is to say, the diffractive optic size was matched to the size of the beam. For example, with a 10 μm feature size, a single 50 x 50 diffractive optic was 500 x 500 μm. Thus, in order to ensure that the entire beam was captured, the images were tiled at least 6x for a final image size of 3000 x 3000 μm.

In the studies involving the direct method, only two levels were considered. That is to say, the images were truncated to 0 and 180°. In addition, this algorithm assumed a uniform planar wave.

For the studies involving the designs based on the annealing method, a proprietary algorithm developed by Hitachi was used. In this case, a 512 x 512 bit map was used, and the final design calculated a diffractive optic with four levels (0, 90, 180 and 270°). Because of the size of the resulting images (512 x 512), tiling was not required. Also, it assumed a non-uniform beam. In this case, a Gaussian beam distribution with a 3 mm diameter was assumed as the illumination. Thus, it was anticipated that DE’s fabricated with these designs should perform better than those fabricated from the direct method because of:

1) High bit resolution (512 compared to 50)
2) Greater number of levels (4 compared to 2)
3) Better approximation of illumination (Gaussian compared to uniform)
Overall two designs were studied:

1) Circle
2) Box

Based on the two diffractive image predictions (direct and annealing), three masks were produced and evaluated:

1) Printed on standard transparency film at 3800 DPI (30 μm features, 2 level)
2) Printed on ultra-clear transparency film at 9600 DPI (20 μm features, 2 level)
3) Chrome on glass mask, professional mask (10 μm features, 2 and 4 level)

Only in the case of the 3rd mask (Chrome on glass), was a 4 level designed considered. In masks #1 and #2, only two level designs were considered. In order to evaluate a two level design from a four level design, only one of the four levels (zero level) was used from the annealing design.

In order to fabricate a four level design from a single mask (Mask #3), a concept known as a rotating mask was used. In this case, all four images required to make a four level design were printed on the same chrome/glass mask. Each image was sequentially rotated 90° and placed concentrically on the center of the mask at 90° orientations. For example, Figure 2.12, shows how the four images (levels 1=A, 2=B, 3=C and 4=D) are orientated and located on the mask so that, when transferred to the wafer, it allows the four images (depths) to be properly superimposed. It is important to note that only the
images location in the quadrant #1 have the proper sequence of etching depths. In addition, during the first etching and the mask was in the #1 position, the etch depth was 1.204 μm. This produced the two level optical elements. In this position, the regions where the four level designs are located, were protected by the photoresist and thus no etching was done. In the other positions, the locations where the two level designs were located where coated with photoresist and accordingly not etched. In addition, the etch depths of the remaining positions were 0.602 μm, 1.204 μm and 1.807 μm respectively.

Figure 2.12 Concept of rotating mask
The actual layout of the rotating mask is shown in Figure 2.13. In this case, only selected locations of diffractive optics are detailed; in fact, all the transparent boxes are either filled with diffractive images or alignment marks.

![Figure 2.13 Layout rotating mask](image)

It is important to note that with the concept of a rotating mask, not only is it important to rotate the diffractive optic images, but also the alignment marks must be rotated from adjacent quadrants. For example, Figure 2.14 (A) shows the orientation of alignment marks in the quadrant #2, and figure (B) shows the marks from quadrant #3. It is seen that markers in (B) are rotated, so that when the mask is rotated during a sequential etching, the marks have the proper orientation.
The diffractive optics were fabricated on a 100 mm diameter wafer that was 1 mm thick. In order to determine the proper etch depths, Figure 2.15, shows the desired etching depth as a function of wavelength for fused silica [42]. It is seen that for a wavelength of 1084 nm, the proper depth is approximately 1200 nm. When four level designs were used, multiples of this depth were used. That is to say, multiples of 0, ½, 1 and 1½ of the 1200 nm were used for the four level designs and only multiples of 0 and 1 of the 1200 nm were used for two level designs.
Each of the fabrication steps for the 100 mm wafer are detailed below.

CLEANING. Usually, a substrate is placed in a strong heated acid bath, such as Piranha (H₂SO₄ + H₂O₂ 1:1 @ 80°C), for a predetermined length of time to remove any organic materials (such as oil) that might reduce surface energy and surface adhesion. Often, this same cleaning procedure is used to remove the photo resist after etching. In addition, often the wafer is dehydrated to remove water vapor. Adhesion promotion is typically completed in a pressure/vacuum oven with hexamethyldisazane (HMDS).
SPIN COATING. In order to assure an uniform coating of the photo resist, a substrate, usually a disc-shaped wafer, is placed on a vacuum chuck and spun at various angular velocities. Initially, a predetermined amount of photo resist is dispensed near the center of the wafer, while the wafer rotates at a relatively low angular velocity (~few hundred RPM). Once the wafer is fully coated by the photo resist, the angular velocity is increased to remove excess photo resist. A typical thickness of a photo resist is 1 to 5 μm, while thicker coating (+10 μm) can also be used. Afterwards, the photo resist is typically baked on a hot plate or in an oven to remove residual solvent.

ALIGNMENT OF MASK. If a single etching is used (two level, top un-etched surface and etched surface) this step usually involves bringing the mask in direct (soft or hard, meaning low or high forces) or near contact (proximity mode) with the wafer, with the only critical dimension being the parallelness of the wafer and the mask. In multiple etchings, it is often critical that the mask (usually a separate mask is needed for each etching step) is oriented in all three dimensions, x, y and ζ direction, where ζ is the angle of relative rotation. In this case, alignment markers are added to the mask and also etched into the wafer for future reference points. A stereomicroscope is then used with a precision movement table to provide relative alignment between the mask and wafer.

EXPOSURE. Once the mask and wafer are properly aligned, the assembly is exposed to UV in order to initiate a photo-chemical reaction in the photo resist. If a positive photo resist is used, the resulting final image will correspond to the image on the mask. That is to say, dark regions on the mask correspond to unexposed regions on the wafer where the
photo resist remains. While there are many commercially available types of positive photo resist, most common is a DNQ chemistry (such as SPR-220) where UV radiation activates photo-acid initiator dye to make it base soluble. In contrast, a typical negative photo resist cross links during exposure so that it becomes a thermoset and becomes less sensitive to solvents. In some cases, the photo resist must be heat treated in an oven or on a hot plate prior to development (cured).

DEVELOPMENT. Once the photo resist has been exposed and cured, it is usually placed in a solvent for a predetermined length of time to remove the uncured photo resist. This is followed by a water rinse and air drying to prevent over development.

ETCHING. There are many types of etching used in the micro-fabrication industry; however, for fused silica there are two primary techniques, HF (Hydrofluoric Acid) and RIE (Reactive Ion Etching). With HF etching, the wafer and photo resist are exposed to hydrofluoric (HF) acid for a pre-determined length of time. Usually, a second wafer (dummy) is used to allow the etching rate to be determined so the final etch depth is correct. The HF selectively etches the wafer in the regions unprotected by the photoresist. It is important to note that in most etching techniques, including RIE etching, some of the photo resist will also be etched. Thus, it is important to ensure that the thickness of the photo resist is sufficiently thick to protect the wafer during the entire etching cycle. Beyond its relative health hazard, the main disadvantage to HF etching of fused silica is that it is an isotropic etching, see Figure 2.16. That is to say, etching occurs in all directions. This results in non-vertical etching, which is detrimental to the function of
DE’s. In contrast, RIE etching typically produces vertical walls with less than 2-3° of draft, see Figure 2.17. In this case, gases such as CHF₃, CF₄ and O₂ along with buffer gases (He or Ne) are ionized with a radio frequency high voltage electric field. Ions are directed at the surface due to difference in surface area of the counter electrodes (smaller electrode) to the chamber electrode (larger electrode). The anisotropy (vertical etching) is due to high field strengths directing neutral atoms at the surface leading to combined sputtering and chemical reactions.

![Figure 2.16 HF etching and isotropic etching](image1)

**Figure 2.16 HF etching and isotropic etching**

![Figure 2.17 RIE etching and an-isotropic etching](image2)

**Figure 2.17 RIE etching and an-isotropic etching**
If more than one etching depth is required, the above detailed steps are repeated as needed, see Figure 2.18.

![Example of multiple etchings](image)

Figure 2.18 Example of multiple etchings

The fused silica wafers were cleaned in concentrated sulfur acid and concentrated hydrogen peroxide at 100°C for 30 minutes before lithography (piranha cleaning). Once cleaned, Figure 2.19 shows the general steps for wafer lens fabrication.
Figure 2.19 Fabrication step of diffractive optic
After piranha cleaning, the wafer was oven baked at 150°C for 30 minutes in hexamethyldisilazane (HMDS) in order to promote adhesion of the photoresist to the wafer.

The photo resist was SPR220-7.0 and was deposited with a thickness of 10 μm. The procedure for spin coating is detailed in Table 2.3.

<table>
<thead>
<tr>
<th>Tool</th>
<th>Speed (RPM)</th>
<th>Accel. (PRM/s)</th>
<th>Spin/Temp</th>
<th>Process time (s)</th>
<th>Exhaust (%)</th>
<th>Disp. Needle</th>
<th>Syringe Press. (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spin</td>
<td>150</td>
<td>100</td>
<td>application</td>
<td>8</td>
<td>0</td>
<td>16 Gage</td>
<td>0.207</td>
</tr>
<tr>
<td></td>
<td>1600</td>
<td>500</td>
<td>spread/thin</td>
<td>60</td>
<td>25</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hotplate</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td></td>
<td>115</td>
<td></td>
<td></td>
<td></td>
<td>30</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>115</td>
<td></td>
<td></td>
<td></td>
<td>90</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 2.3 Details of spin coating procedure

Once the wafer was coated, it was soft baked at 95 °C for 90 seconds on a hot plate in N$_2$ gas atmosphere. In the aligner, a dummy (Silicon) wafer was placed under the sample to prevent reflected UV bleeding through the clear fused silica wafer. The wafer was then exposed to UV radiation for 3 s at a density of 15 mW/cm$^2$. The wafer was then developed for 2 minutes and water rinsed followed by a spin dry.

In the majority of the work, a LAM 490 unit (LAM and Associates) was used for reactive ion etching of the wafer. Table 2.4 details the procedure for reactive ion etching. This
procedure was repeated 4 times. As seen in the table, step #2 (the etching step) was varied during according to desired etch depth.

<table>
<thead>
<tr>
<th>Process</th>
<th>Step 1</th>
<th>Step 2</th>
<th>Step 3</th>
<th>Step 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure (Torr)</td>
<td>2.6</td>
<td>2.6</td>
<td>2.6</td>
<td>2.6</td>
</tr>
<tr>
<td>RF (W)</td>
<td>0</td>
<td>600</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Gap (mm)</td>
<td>0.38</td>
<td>0.38</td>
<td>0.38</td>
<td>1.35</td>
</tr>
<tr>
<td>Argon</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>O₂</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>He</td>
<td>120</td>
<td>120</td>
<td>120</td>
<td>120</td>
</tr>
<tr>
<td>CHF₃</td>
<td>40</td>
<td>40</td>
<td>40</td>
<td>40</td>
</tr>
<tr>
<td>CF₄</td>
<td>45</td>
<td>45</td>
<td>45</td>
<td>0</td>
</tr>
<tr>
<td>Time</td>
<td>1:00</td>
<td>Depth dependent</td>
<td>0:10</td>
<td>0:10</td>
</tr>
</tbody>
</table>

Table 2.4 Details of RIE procedure

One lens (wafer) was fabricated on a table top RIE unit (Technics Micro-RIE Series 800 II). This unit is limited to 350 W and only allows two gases for plasma generation. The gases and flow rates were CF₄ and Argon at 30 and 15 cm³/min, respectively. The pressure was set at 40 to 60 mTorr.

2.2.3 DIFRACTIVE OPTIC WELDING AND CHARACTERIZATION

In the majority of welding experiments with diffractive optics (both computer generated and holographic), an 80 W fiber laser was used (IPG Photonics YLR-100). The wavelength was 1084 nm and the raw beam had a diameter of approximately 5 mm.
Various configuration were studied, including illumination with the raw beam; however, the best results were obtained with the configuration shown in Figure 2.20.

Figure 2.20 Layout for welding with diffractive optics

In most welding configurations, the 0 order (hot spot) coincided with the hole drilled into the absorbing sample for application of compressed air during burst testing, see Figure 2.11. If an alternative setup was used, the 0 order was masked with a glass slide coated with a circular film of copper (3 mm diameter). The center of the copper circle was aligned with the center of the 0 order. The mask was placed as close to the weld plane as possible in order to reduce energy losses.
In most cases, the transparent bladder [43] was used to ensure that intimate contact was maintained during welding. The pressure was held constant at 0.25 MPa. The welding parameters that were studied were:

1) Power  
2) Time  
3) Working distance

Weld quality was measured by evaluating the strength of the welds as well as visual inspection of weld fidelity relative to the desired image.

In order to measure the efficiency of the diffractive optics (computer generated), power was measured with three configurations:

1) Power into the diffractive optics (Figure 2.21 (A))  
2) Power in 0 (Center hot spot) and 1st order (desired image) (Figure 2.21 (B))  
3) Power only into 1st order (desired image) (Figure 2.21 (C))

In this experimental setup, the higher order diffraction patterns fall outside the window of the power meter and thus masked by the housing of the power meter.
The overall efficiency of the diffractive optic ($Effec$) was then calculated as:

$$Effec = \frac{P_1}{P_T}$$  \[2.5\]

Where $P_1$ is the power in the first order (Figure 2.21 (C)) and $P_T$ is the total power delivered to the diffractive optics (Figure 2.21 (B)). This also allowed the power lost in the 0 order to be measured. In addition, by measuring the losses in the transparent
bladder, the power delivered to the weld zone was measured. It is important to note that in the majority of the reported data, the reported power is the true delivered power and accounts for the losses in the undesired orders as well as losses in the transparent bladder and sample.

In order to gain insight into the power distribution within the cross section of the diffractive image, a knife edge beam characterization [44] technique was used. The process basically works by slowly moving a knife edge that is parallel to a line segment and measuring the power as a function of edge location. In this study the 0 order was masked near the diffractive image in order to prevent equipment damage. The knife edge was a razor blade and it was positioned with a micrometer.

![Figure 2.22 Layout of knife edge experiments](image)

Figure 2.22 Layout of knife edge experiments
The derivative as a function of position was taken in order to calculate actual power density.

### 2.2.4 BURST PRESSURE MEASUREMENTS

Pressure burst testing was evaluated as an alternative to tensile testing because of the inherent weld geometry. Air pressure was applied to the weld sample through the hole so that the cavity between the clear sheet and the black sample was inflated. Figure 2.23 shows a cross-sectional view of the experimental setup. An aluminum block was machined with a manifold design so that air pressure from a proportional valve was directed to a pressure transducer and to a port where the sample was adhesively bonded. The samples were adhesively bonded to the fixture plates with “Krazy®” Glue. Care was taken to ensure that the entire surface between the black sample and the aluminum manifold was fully coated to provide a hermetic seal.
The pressure was varied using a SMC (model VEP312) proportional valve. This particular model was selected because of its availability. In order to apply a linearly increasing pressure to the sample, an integrator circuit was designed and built (see Figure 2.24). It was believed that it was critical that a constant and repeatable rate of loading be applied to the samples because plastics are load-rate sensitive. The output voltage from this circuit was then applied as the control voltage signal to the proportional valve amplifier. The rate of the pressure increase was held constant at 5.71 kPa/s. At this rate, most samples failed during a test cycle between 20 and 120 s.
The pressure was measured using an Omega PX26-100DC pressure transducer. A Sensotec In-Line-Amplifier (060-6827) was used to amplify the signal from the pressure sensor. The data from the pressure transducer was recorded with a PC-based data acquisition system at a sampling rate of 90 sample/s. The ultimate pressure required to initiate a leak or fracture of the weld was recorded as the weld strength (burst pressure).
2.3 RESULTS WITH DIFFRACTIVE OPTICS

2.3.1 DIFFRACTIVE OPTIC CHARACTERISTICS

2.3.1.1 DIFFRACTIVE OPTIC IMAGES

Figure 2.25 shows diffractive patterns for the circle that was generated with the direct algorithm methodology. In the first image (A), a single pattern is shown and in the second image, the same pattern has been tiled 5 x 5 times. Because the direct method only predicted two level designs, each level is represented by black or white. It is important to note that, because only two levels/phases are used, it is irrelevant whether the black or white areas correspond to 0 or 180°, since the two levels will always be 180° out of phase. That is to say, the zero phase (0 level) can be assigned to either 0 or 180°.
Figure 2.26 shows a two level design for a diffractive pattern predicted with the annealing algorithm. It is interesting to note that this image has a pattern that appears to have symmetry about the center of the pattern, which is due to the fact that this algorithm accounts for a Gaussian distribution, which has a higher energy density at its center. This is in contrast to the patterns seen in Figure 2.25, where a uniform planar wave is assumed in the algorithms.
Figure 2.26 Diffractive image for circle pattern (512 x 512-anneal design), two level only

Figure 2.27 shows a similar pattern, except that a four level design is shown. Unlike the two level design, where phase to darkness relationship is not critical, the phases must be properly matched. In this case, the phases/level correspond to darkness. That is to say:

Darkest pixels=0°
Dark pixels=90°
Medium pixels=180°
Lightest pixels=270°
Figure 2.27 Diffractive image for circle pattern (512 x 512-anneal design), four levels

For reference reasons, Figure 2.28 shows a diffractive pattern generated with the annealing algorithms for the square image. Again, it is seen that there appears to be symmetry about the center of the pattern.
2.3.2 DIFFRACTIVE OPTIC ETCHING RATES

Because the table top RIE had relatively low plasma power (350 W) and only allowed two gasses for the plasma, it was found that its etch rate was only 0.002 μm/min.
Because of equipment limitation, the longest etching time was 170 minutes. While it was anticipated this would result in under-etched features, the element was evaluated for reference purposes.

For most of the work the LAM RIE was used. Figure 2.29 shows etch rate as a function of time based on a measurement on a control wafer. The feature depth measurements were done using a standard profilometer (Solarius Ditech). It is seen that the etch rate is time- (depth-) dependent. This is expected because with increasing feature depth, there is less freedom of movement of the ions for etching and they lose their moment (energy).

![Figure 2.29 Etching rate as a function of time for LAM RIE](image-url)
A quadratic curve fit for the etch rate \((dz/dt \ (\mu m/min))\) as a function of time gives:

\[
\frac{dz}{dt} = -0.0034t^2 + 0.0228t + 0.2846 \quad [2.1]
\]

It is seen that Eq 2.1 is a standard differential equation, with a solution as shown in Eq 4.2 with the initial condition that at \(t=0\) \(z=0\).

\[
z(t) = -0.001133t^3 + 0.0144t^2 + 0.2846t + 0.012 \quad [2.2]
\]

This allows the estimation of etching time in order to achieve a final etch depth \((z)\).

### 2.3.3 DIFFRACTIVE OPTIC SURFACE/ETCHING QUALITY

As previously discussed, the initial fabrication of a diffractive element used a standard overhead transparency as a mask. The diffractive image was printed at a resolution of 3800 dpi and the feature sizes were designed for 30 \(\mu m\). Figure 2.30 shows a SEM (scanning electron microscopy) image of the final lens. It is important to note that the lens was pre-coated with a thin layer of silver in order to prevent electrical buildup on the non-conductive wafer. There are three major observations that can be made from these images, namely:
1) The over-all pattern was well replicated. This is seen in the fact that at the lower magnification, the pattern appears to be correct.

2) There is significant surface roughness in the etched patterns (high magnification). Because a positive photoresist was used, these regions correspond to regions where the wafer was not protected by the photoresist, or regions where the mask is clear. In contrast, the un-etched regions are areas where there is ink printed on the mask, which protected the photo resist from the polymer chain sectioning UV radiation. While the transparency appeared relatively clear, small particles embedding in the film caused scattering of the UV light, which in turn caused local under-exposure of the photoresist. Attempts were made to over-expose the photo resist during the alignment procedure; however, other issues, such as loss of feature resolution, resulted from the over-exposure.

3) The features appear under-etched and do not have the proper depth, as seen in the high magnification picture.
In order to confirm the observation that the features were under-etched, AFM (atomic force microscopy) was also performed, see Figure 2.31. As shown in the down-looking view (the lower left image), the features appear relatively irregular; however, because of the scaling of the images, these irregularities are minimal as depicted in the SEM. More importantly, the AFM images show that the final etch depth was only 407.6 nm, despite the ideal depth being 1204 nm. This is an under-etch of 786.4 nm or 66.1%. This is the result of the lack of a proper etching rate being limited by the table top RIE.
Figure 2.31 AFM cross section of element fabricated with table top RIE and overhead transparency mask

Figure 2.32 shows an AFM image of the element fabricated with the ultra-clear transparency. The picture in the upper left corner of the figure shows a small portion of the diffractive pattern where only two levels are depicted. Each level is represented by separate colors/darkness’s. It is seen that the surface roughness is very smooth. This evident by the fact that the distribution of the depths (upper left hand image) has only two corresponding colors. In addition, by referring to the histogram of the depth measurements (image on right side of figure), it is seen that there are only two well
defined levels, one at 80 nm and a second and 1286 nm. The histogram is based on the depth distribution within the rectangle defined in the upper left hand image. Thus, the overall feature depth is 1206 nm which is only 2 nm from the targeted depth of 1204 nm (error=0.17%). Thus, it is seen that by using better mask (ultra-clear transparency) and better controlled RIE, the desired feature depths and surface smoothness is achievable.

Figure 2.32 AFM cross section of element fabricated with table LAM RIE and ultra-clear overhead transparency mask
The final element that was evaluated was one that was also fabricated with the LAM RIE, but with the chrome on glass mask. The major difference compared to the previous element is that this element had four levels, thus alignment of existing features relative to the mask is critical. Figure 2.33 shows an AFM three-dimensional contour plot of a portion of the element. Four separate levels can be seen (including the top surface). However, it is also seen that despite best efforts, there was some misalignment during one of the etching steps. This misalignment is evident by the relatively narrow tall walls. In this case, the misalignment was less than 1.5 μm and was considered acceptable. In addition, as previously reported, the surface smoothness also appears acceptable.

Figure 2.33 AFM contour plot of element fabricated with LAM RIE and chrome on glass mask
Figure 2.34 shows a cross sectional AFM image of the same element. The final etch depths, phases and corresponding errors are detailed in Table 2.5.

<table>
<thead>
<tr>
<th>Desired depth (nm)</th>
<th>Phase (deg)</th>
<th>Actual depth (nm)</th>
<th>Absolute error (nm)</th>
<th>Relative error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>602.2</td>
<td>90</td>
<td>560.1</td>
<td>-42.1</td>
<td>-7.0</td>
</tr>
<tr>
<td>1204</td>
<td>180</td>
<td>1239</td>
<td>35</td>
<td>2.9</td>
</tr>
<tr>
<td>1807</td>
<td>270</td>
<td>1783</td>
<td>-24</td>
<td>-1.3</td>
</tr>
</tbody>
</table>

Table 2.5 Details etch depths with four level design and LAM RIE

It is seen that the depths are very close to the desired depths and the deviations from the desired values were considered acceptable.
Figure 2.34 AFM cross section of element fabricated with LAM RIE and chrome on glass mask

Figure 2.35 shows an SEM of an element fabricated with the LAM RIE and the chrome on glass mask. It is seen that the surface quality of the etch is relatively smooth. That is to say, there are no pits as seen in Figure 2.30.
2.3.4 DIFFRACTIVE OPTIC ELEMENT CHARACTERIZATION

Three basic characteristics were quantified for the various elements that were fabricated, namely;

1) Divergence of image
2) Efficiency of element

Based on Eq. [2.1] \( (y = \frac{m \lambda D}{d}) \), the predicted image divergence was measured. It is seen that the predicted and actual values are in good agreement. That is to say, the larger the distance between the diffractive optic and the image plane (weld distance), the larger the image.
Using the experimental setup depicted in Figure 2.21, the efficiencies of two elements were measured. It is important to note that the efficiencies are the energy delivered to the 1st order image only (desired image) divided by the energy into the diffractive optic (Eq. [3.2]). The two elements included:

1) Two level element (direct algorithms)

2) Four level element (bi-directional algorithms)
Based on the initial cycle times (greater than 10 s) and power levels (80 W into element) required to make burn patterns on the ZAP paper, the efficiencies of the element fabricated with the table top RIE were not measured because it was assumed to be very low (-5%).

Figure 2.37 shows the efficiencies of the various elements that were measured. It is seen that the efficiencies of the two level (direct algorithm) element is 50.5%. It is also seen that the four level element has an efficiency of 59%.

![Figure 2.37 Measured efficiencies of various elements](image.png)
In order to gain insight into the power distribution within the cross section of the diffractive image, a knife edge beam characterization technique was used. In this experiment, the 2 and 4 level designs were studied and the box image was selected. The box image was selected because it allows three of the four line segments to be mask from the power meter during the experiment as well as allowing the remain segment to be parallel to the knife edge.

As shown in Figure 2.38 the power distribution for both element design is relatively non-uniform. The two level design has a distribution that is nearly a Gaussian, as expected. In addition the four level design appears to have higher orders of diffraction which is also expected, however, the distribution is not symmetrical. It is expected that this is caused by the experimental error in element fabrication, namely offset of the various levels during mask alignment.
2.3.5 DIFFRACTIVE OPTIC WELDING

During the initial experiments, a YAG laser was used because of equipment resource reasons (Spectra Physics, 50W Tornado). In this case, the wavelength was 1064 nm. In addition, in the initial study, the element fabricated with table top RIE was used with the circle image. Figure 2.39 shows photographs of welds made in the initial evaluation at various times (10 to 20 s). The outer diameter of the welds is approximately 14 mm. In these studies, the output of the laser was 45 W and because of the low efficiency of the element (not measured) it is seen that long cycle times were required to make welds. Despite the fact that the element was of very poor quality (poor design and poor fabrication), a distinctive circular pattern was welded.
Figure 2.39 Welds made with element fabricated with table top RIE and overhead transparency mask (2 level)

Figure 2.40 shows a burn pattern on ZAP paper (A) and a weld made in 2 s with a 2 level element fabricated with the LAM REI and from the ultra-clear transparency. It is seen that images are relatively clear. That is to say, the individual pixels from the original circle design (art work) can be seen, especially in the ZAP paper image. It is also seen that two circles slightly offset from each other are projected by the element. Two circles are produced because in the original art work, the circle was not perfectly centered in the image array. It is important to note that in these (and all further detailed experiments) the fiber laser (1084 nm) was used.

Figure 2.40 (A) Zap paper image and (B) weld (2 s, 37 W) made with 2 level element fabricated with LAM RIE and ultra-clear overhead transparency mask
Figure 2.41 shows similar photographs for the box image. Again, it is seen that the weld was generated in a relatively short time period (2 s). However, the corners of the box image did not fully weld. In addition, in the ZAP paper image, the mask for the 0-order can be seen and there is some energy distributed around outer edges of the mask that was not fully removed.

![Figure 2.41 (A) ZAP paper image and (B) weld (2 s, 37 W) with 2 level element fabricated with LAM RIE and ultra-clear overhead transparency mask](image)

Figure 2.42 shows a weld and predicted image using the four level element with the chrome on glass mask (best element). The outer diameter of the circle in this case was 20 mm. It is seen that the weld image is very similar to the predicted image. Despite the fact that the weld width varies, the circle is fully welded. In addition, the cycle time is relatively short (0.5 s).
Figure 2.42 (A) weld (0.5 s, 47.2 W) with 4 level element fabricated with LAM RIE and chrome on glass mask.

Figure 2.43 shows weld made with box image with the two level design. It is seen that the welds are relatively uniform and with cycle times greater than 2.0 s, the box image is fully welded. In this case, the laser output was 60 W.

Figure 2.43 Welds made with 2 level element fabricated with LAM RIE and chrome on glass mask (2 level design).
Additional welds were made with the circle design in order to determine the minimal weld widths. These welds were made with the element fabricated with LAM RIE and chrome on glass mask (4-level) at a relatively short weld distance (125 mm), in order to produce a weld circle with a diameter of 10 mm. The cycle times were varied between 0.025 s and 0.2 s and the weld power was 47.2 W. Figure 2.44 shows the results from these studies. As expected, weld width is proportional to weld time. However, most importantly, it is seen that the minimum weld width is as narrow as 115 μm with a weld time of 25 ms.

Figure 2.44 Weld widths of circle image (OD=10 mm) with 4 level element fabricated with LAM RIE and chrome on glass mask
Figure 2.45 shows a micrograph of selected regions of the weld made with a 10 mm diameter. It is seen that there is evidence of fractures near the outer diameter of the welds. It is believed that this is primarily the result of residual stress relaxation due to relatively short cycle times (25 ms) and high power dissipation (47.2 W). It is believed that process optimization may reduce these stresses. It is also seen that at longer weld times, there is a region in the center of the weld that appears under-welded. Based on power distribution detailed in Figure 2.38, this under-welded region corresponds to the lower power density region in the center of the beam. It is also seen that there is variation in weld widths with the larger circle. Again, suggesting that the diffractive pattern was not fully optimized.
Circular welds made with a diameter of 20 mm were burst tested as detailed in Section 2.2.4. Again, these welds were made with the 4 level element fabricated with LAM RIE and chrome on glass mask. Figure 2.46 shows the pressure profile for various welding conditions. It is seen that the pressure increases in a linear fashion. It is also seen that at higher energy inputs (47.2 W for 0.5 s), the weld never failed. That is to say, the weld was able to sustain the maximum test pressure (650 kPa). At lower energy levels (29.5 W for 0.5 s), the welds did fail. In all cases, the failure was catastrophic (sudden).

Figure 2.46 Typical pressure profiles for two welding parameters
Figure 2.47 shows the burst pressure as function of weld time for two power levels. It is seen, as expected, that burst pressure is proportional to weld time and weld power. It is important to note that the reported power is the true power to the weld and accounts for all power losses in the optical system. It is important to note that the maximum pressure of the experimental setup was 0.67 MPa. Thus, burst strengths above this pressure were not tested. For example, at the lower power level (29.5 W), weld times greater than 0.8 s resulted in samples that did not fail, so the maximum pressure of 0.67 MPa was recorded for these samples.

Figure 2.47 Burst pressure as a function of weld times for two power levels (20 mm OD)
Figure 2.48 shows the same data, except that the data is normalized to weld energy. As expected, it is seen that burst pressure is proportional to weld energy over the testable range (< 18 J, 0.67 MPa).

Figure 2.48 Burst pressure as a function of weld energy (20 mm OD)
2.4 DIFFRACTIVE OPTIC WELDING OF COMPLEX SHAPES

In order to ensure that complex shapes could be welded using diffractive optic, a diffractive optical element to produce the text “OSU” was designed and fabricated. Figure 2.49 shows a typical burn pattern and weld using the diffractive optic. It is seen that while the image quality is not perfect and there is some non-uniformity, the general image is relatively good.

Figure 2.49 (A) Burn pattern on ZAP paper and (B) weld on PC with the text “OSU”
CHAPTER 3

HOLOGRAPHIC OPTICS

3.1 HOLOGRAMS

Holograms are a special type or group of diffractive optics. The main difference between diffractive optics and hologram is the field of focus. Diffractive optics form images in 2 dimensions while in contrast holograms produce images in 3 dimensions.

3.1.1 FUNCTIONALITY OF HOLOGRAPHIC OPTICS

Holograms are a special type of diffractive optics. They have been used for many years for entertainment to produce interesting 3-dimensional images. For example, Figure 3.1 shows a typical holographic image. When viewed properly, by illuminating the holographic film with a collimated beam of light at the correct angle, a 3-dimensional image is produced.
There are three main differences between holograms and typical diffractive optics, as discussed in the previous sections:

- Holograms are typically produced by photographic techniques instead of computer algorithms.
- Holograms are commonly used to generate 3-dimensional images, while diffractive optics typically (not always) generate 2-dimensional images.
• Holograms are continuously varying patterns while diffractive optics have discrete varying patterns.

While holographic patterns can be generated by computer algorithms that can produce 3-dimensional images, because of intensive computational requirements, they are more commonly produced using photographic/optical techniques. In general, there are two major types of holograms, the transmission type and the reflective type [46]. The most common type of hologram is the reflective type, as commonly seen on credit cards for security reasons. As the name implies, in a reflective type hologram, the interference of reflected light from a diffractive pattern produces an image. In contrast, transmission holograms produce an image by interference of light that passes through a diffractive pattern. The light that passes through the image superimposes with the reference beam and produces the diffraction pattern. A typical transmission hologram has a diffractive pattern that consists of clear and dark regions, similar to a computer generated magnitude diffractive element, except that the pattern is very complex. As previously detailed, a magnitude diffractive pattern absorbs approximately 50% of the light and thus is relatively inefficient. By bleaching the holographic film (a secondary chemical development step), it is possible to alter the film and change the clear and dark regions into varying indexes of refraction, so that the hologram effectively becomes a phase diffractive element. This can greatly increase the efficiency of the hologram.
3.1.2 FABRICATION OF HOLOGRAPHIC OPTICS

As previously detailed, holograms are typically fabricated by a photographic technique. The technique involves illuminating a real object with a beam of light that is spatially coherent to a reference beam. The reflected light is then directed at photographic film that typically has 2500 lines/mm of resolution. In more detail, as seen in Figure 3.2, a laser beam is split into two beams. One beam is passed through a beam expander (telescope) and directed onto photographic film with very small grains sizes (<5 μm). The beam expander only increases the diameter of the beam while maintaining the beams collimation. The second beam is also expanded, but its collimation is not critical. The expanding beam is then directed at the object of interest. The object, film, and beam are positioned so that the resulting reflection from the object is primarily directed to the film. In addition, the optical components are also configured, so that the travel distances for both beams from the beam splitter to the film are equal within the spatial coherency length of the laser. That is to say, referring to Figure 3.2, distances \((A1+A2+A3) \sim (B1+B2)\). In this configuration, the differences in the travel distances of the two beams is equal to the topographic features of the object. These differences then result in the two beams superimposing upon each other at various phases. This results in some regions that have destructive interference and other regions that have constructive interference. This results in alternating dark and bright regions of light being exposed on the film.
In addition, the beam splitter is adjusted so that the light from the beam expander (B2) is approximately 3 times in intensity compared to the light from the object (A3). This ensures that the superposition of the two beams is always positive. That is to say, the superposition of the two beams never produces totally dark regions, but only relatively light regions. It is also important to note that the intensity of both beams must be measured and the exposure time adjusted accordingly to match the exposure of the film. It is usually best to reduce the exposure time to a minimum by using a relatively high power laser (>200 mW) in order to reduce vibrational effects. Vibrations of the film, object, or optics can result in variations of the distances that the split beams travel and it will alter the diffractive pattern and reduce the quality of the final hologram.

Figure 3.2 Typical experimental setup to produce a holographic film
3.2 EXPERIMENTAL PROCEDURES WITH HOLOGRAPHIC OPTICS

Two objects were used to encode a holographic image:

1) Reflective circle (20 mm dia, 3 mm line width)

2) Transmission circle (20 mm dia, 3 mm line width)

The reflective object was a white circle printed on a black background. The transmission object was fabricated on a clear sample of glass (200 x 300 mm x 2.5 mm) painted black with a circular pattern remaining clear (no paint). The glass was grit blasted prior to painting in order to provide a diffuse image. Figure 3.3 shows a photograph of the transparent object mounted in anti-vibration holder.

Figure 3.3 Photograph of transparent object in holder
A 100 mW He-Ne laser was used as laser source for the encoding. Figure 3.4 shows the experimental setup for the beam path and significant optical components. In this figure, the setup was used the transparent object. The exposure times was set at 10, 30 and 60 seconds. The film was standard holographic film from JD-2 from Integraf®. The beam was expanded to approximately 100 mm in diameter. The film was developed following the procedures detailed by the manufacturer. The basic development procedure was:

- Place film in developer solution for 20 s
- Rinse in water for 20 s
- Place in bleach for 10 s
- Rinse in water for 20 s
Figure 3.4 Photograph of holographic encoding setup
3.2.1 HOLOGRAPHIC WELDING

In order to fully illuminate the hologram and with the laser beam from the fiber laser, the beam was expanded to match the diameter of the reference beam (~7.5 cm). This was accomplished with selected lens as shown in Figure 3.5.

![Figure 3.5 Experimental setup for welding with hologram](image)

The output power of the laser was varied from 0 to 80 W and the heating time was varied from 0-20 s. In selected experiments, ZAP paper was in replacement of the weld sample in order to determine weld fidelity. The location of the image was determined using an IR sensitive camera.
3.3 RESULTS AND DISCUSSION WITH HOLOGRAPHIC OPTICS

3.3.1 HOLOGRAM SURFACE/QUALITY

Figure 3.6 shows a photograph of a portion of the hologram fabricated with the transparent object. It is seen that the diffractive pattern appears to be very random. The individual spots are approximately 2-5 μm in size. The black objects are simply dirt.

![Figure 3.6 Micrograph of hologram](image)

3.3.2 HOLOGRAM CHARACTERIZATION

Using the same laser (HeNe-530nm) used to encode (produce) the holographic film, the image quality of the circle pattern was relatively good as shown in Figure 3.7. While there appears to be slightly more energy directed to the lower right hand side of the circle, it is relatively uniform. Because the beam could not be obstructed, the photograph was taken at an angle, which caused the circle to appear slightly oval.
Using a similar technique to the one detailed in Section 2.2.3, it was found that for the HeNe laser the hologram was approximately 70% efficient.

However, when the same hologram was used with the fiber laser (1084 nm), the results were less promising. The efficiency was so low that accurate measurements were not obtainable. It is estimated that the efficiency was less than a few percent. In addition, it was found that the image was produced at a large angle relative to the hologram (see Figure 3.8). For example, when the hologram was illuminated with the HeNe laser, the image would form at approximately 25° from the normal relative to the hologram. This corresponded to the location/angle of the object relative to the film during encoding. However, when the same hologram was illuminated with the fiber laser, the image would be produced at approximately 45° from the normal relative to the hologram, Figure 3.8.
It is important to note that during these experiments the laser beams were expanded to approximately 100 mm in diameter in order to use the entire encoded holographic image. Because of the low efficiencies, it was never possible to produce a weld with the holographic lens and, in addition, patterns on ZAP paper took as long as 10 s at 80 W of illumination. As seen in the ZAP paper image in Figure 3.9, the hologram image was not uniform.
Figure 3.9 ZAP paper image from hologram with fiber laser

It is believed that most of the aforementioned problems with the hologram were caused by the fact that the image was encoded at a different wavelength of laser light than that used to illuminate the hologram. Because there are no commercially available photographic films sensitive to a wavelength of light of 1084nm, no additional experiments with the holographic imaging were performed.
CHAPTER 4

MOLECULAR HEALING

Because a portion of this work was focused on predicting weld size based on thermal histories, temperature histories had to be either measured or predict. In the case of micro-welding, were the welds were much small (<50 μm) than even the smallest thermocouple, thermal histories were based on temperature field predictions. The predictions were based on conventional closed form solutions of various heat source geometries, depending on the welding process. Overall two heat sources were modeled; 1) TTIr scan laser welding and 2) TTIr stationary point laser welding. The following sections detail the heat flow models that were used in this study.

4.1 HEATING MODELS

Two theoretical models were used in this study:

1) Rosenthal’s point heat source [47], and

2) Gaussian distributed heat source
Both the models assume a semi-infinite body. Because the lower samples used in this study were at least 2.5 mm thick, this assumption is valid. However, since the top samples were only 250 μm thick this assumption is only valid by considering the heat flow into the fixtures (glass), see Figure 4.1.

Figure 4.1 Details of model based on experimental setup (moving heat source)

Each of these models is detailed in the following sections.

4.1.1 ROSENTHAL’S MOVING POINT HEAT SOURCE

Rosenthal’s point source theory analyzes the temperature distribution in a semi-infinite plate with a point heat source moving at a constant velocity (see Figure 4.2).
Two coordinate systems are considered, a fixed coordinate system and a moving coordinate system with its origin located on the surface of the plate below the heat source. The moving coordinate system moves at the same velocity \( v \) as the heat source. Neglecting edge effects, this allows the model to be greatly simplified since the problem is reduced to a quasi-steady state heat flow condition. For example, far away from the edges (start and end of weld), the temperature distribution in the moving coordinate system is constant for all times. For example, a point that is 1 cm behind the heat source and moves with the heat source remains at a constant temperature. Relative to the fixed coordinate system, points experience heating and cooling as the heat source passes near any given point. But, since the moving coordinate system is moving with the heat source, points on the moving coordinate system do not experience heating and cooling. In the moving coordinate system, \( w \) is related to the \( x \)-coordinate and is defined as:
\[ w(t) = x + vt \]  

[4.1]

In order to calculate the temperature within the body, it is necessary to consider a control volume, with width \( dw \), height \( dz \) and length \( dy \) (see Figure 4.3).

![Figure 4.3 Details of heat and mass flow in and out of a control volume](image)

Because the control volume for this element is moving with the moving coordinate system, as it translates through the body in the x-direction, there is mass with some internal energy moving in from the right and out to the left of the element. From conservation of energy, the internal energy change results from the net heat flow into the control volume as well as from the internal heat generation rate \((\dot{\theta})\). This net energy balance is given by:
Net \( \Delta \) internal energy = \((q_{in}) - (q_{out}) + \dot{Q}\) (internal heat generation rate)

\[
\rho C \frac{\partial \theta}{\partial t} dydwh = \left( q_w \ dydz \right) - \left( \dot{q}_{w+dw} \ dydz \right) + \left[ \left( \rho C \nu \theta \right)_{w+dw} dydz \right] - \\
\left( \rho C \nu \theta_w \right) dydz \\
+ \left( \dot{q}_y \ dwdz \right) - \left( \dot{q}_{y+dy} \ dwdz \right) + \left( \dot{q}_z \ dwdy \right) - \left( \dot{q}_{z+dz} \ dwdy \right) + Q \ dwdydz
\]

[4.2]

Where \( C \) is specific heat, \( \rho \) is density, \( \theta \) is temperature and \( t \) is time. From Taylor’s series expansion and assuming the density and specific heat remain constant, it is possible to define the following:

\[
\begin{align*}
\dot{q}_{w+dw} &= q_w + \frac{\partial q_w}{\partial w} dw \\
\dot{q}_{z+dz} &= q_z + \frac{\partial q_z}{\partial z} dz \\
\dot{q}_{y+dy} &= q_y + \frac{\partial q_y}{\partial y} dy \\
\theta_{w+dw} &= \theta_w + \frac{\partial \theta_w}{\partial w} dw
\end{align*}
\]

[4.3]

Substituting Eqs. 4.3 into Eq. 4.2, gives;
\[ \rho c \frac{\partial \theta}{\partial t} = -\frac{\partial q_w}{\partial w} - \frac{\partial q_z}{\partial z} - \frac{\partial q_y}{\partial y} + (\rho c v) \frac{\partial \theta}{\partial w} + \dot{Q} \]  \hspace{1cm} [4.4]

In addition, if Fourier’s law of conduction is applied:

\[ q_w = -\lambda \frac{\partial \theta}{\partial w} \]
\[ q_y = -\lambda \frac{\partial \theta}{\partial y} \]
\[ q_z = -\lambda \frac{\partial \theta}{\partial z} \]  \hspace{1cm} [4.5]

where \( \lambda \) is the thermal conductivity of the material. Assuming \( \lambda \) is constant and there is no internal heat generation, then Eq. 4.5 becomes:

\[ \rho c \frac{\partial \theta}{\partial t} = \lambda \frac{\partial^2 \theta}{\partial w^2} + \lambda \frac{\partial^2 \theta}{\partial z^2} + \lambda \frac{\partial^2 \theta}{\partial y^2} + (\rho c v) \frac{\partial \theta}{\partial w} \]  \hspace{1cm} [4.6]

It is assumed that the material properties are constant, which is a poor assumption for plastics, especially near a transition point like \( T_g \) or \( T_m \). For a quasi-steady state case \( (d\theta/dt = 0) \), Eq. 4.6 reduces to:
\[ \frac{\partial^2 \theta}{\partial w^2} + \frac{\partial^2 \theta}{\partial y^2} + \frac{\partial^2 \theta}{\partial z^2} = -\frac{\nu}{\kappa} \frac{\partial \theta_w}{\partial w} \]  

[4.7]

Where \( \kappa \) is the material’s thermal diffusivity:

\[ \kappa = \frac{\lambda}{\rho c} \]  

[4.8]

By defining the distance from the heat source as:

\[ r(t) = \sqrt{w(t)^2 + y^2 + z^2} \]  

[4.9]

and by making the following two assumptions:

1) The heat loss due to convection to air is zero (a valid assumption because in TTIr there is no heat convection). In addition, it is possible to assume symmetry between the clear and black sample, see Figure 4.1.

2) Far from the heat source, the temperature is constant or the temperature gradient is zero, \( \lim_{r \to \infty} \frac{\partial \theta}{\partial r} = 0 \).
For the point heat source, the heat flow through a hemisphere (see Figure 4.4) multiplied by the surface area of the hemisphere must be equal to the power as the radius of the sphere approaches zero:

\[
\lim_{r \to 0} 2\pi r^2 \left( -\lambda \frac{\partial \theta}{\partial r} \right) = P
\]

[4.10]

Figure 4.4 Details of heat flow from a point source through a hemisphere

Rosenthal [47] has shown that it is possible to calculate the temperature at any location within the plate using the following equation:
\begin{equation}
\theta(t) = \theta_0 + \frac{P}{2\pi\lambda r(t)} e^{-\frac{w(t) + r(t)}{2\kappa}}
\end{equation}

Where \(\theta_0\) is the initial temperature of the body.

4.1.2 DISTRIBUTED HEAT SOURCE

Real heat sources cannot be modeled as a point heat source, which led Eagar and Tsai [48] to build on Rosenthal’s model to describe the temperature fields produced by a moving heat source that has a Gaussian type distribution. Before this type of heat source is defined, it is important to describe when a heat source cannot be modeled as a point. A point heat source can be used when the material has a relatively high thermal diffusivity and the heat source is relatively small. In addition, if the material being processed has a relatively low thermal diffusivity, the maximum size of a heat source that can be represented as a point is reduced. While this distinction is vague, it will suffice for the description of a distributed model. Thus, in the case of micro welding of plastics, where the thermal diffusivity is relative low, it is no longer valid to represent the heat source as a point. In the case of a focused laser beam, the heat source most likely follows a Gaussian type distribution. While the actual distribution may vary slightly because of aberrations in optics or issues related to the laser generator, it is possible to define the power distribution (Q) over an area in the x and y directions as follows:
In this case, $q$ is the power from the laser, $x$ and $y$ correspond to the $x$ and $y$ direction respectively and $\sigma$ corresponds to the width of the distribution (distribution parameter).

In more detail, $\sigma$ equals the distance from the center of the heat source to a point where the power distribution is equal to $60.65\%$ ($e^{-1/2}$) of its peak value. As an example, Figure 4.5 shows the power distribution over a given area for two distribution parameter values. It is seen that larger distribution parameters promote a wide distribution of the power.

\[
Q(x, y) = \frac{q}{2\pi\sigma^2} e^{-\frac{(x^2 + y^2)}{2\sigma^2}}
\]

[4.12]

\[\sigma=12.5 \, \mu m \quad \sigma=25 \, \mu m\]

Figure 4.5 Example of Gaussian type heat distribution (dimensionless) for two different distribution parameters with identical power levels
For modeling purposes, it is a simple way to describe the distributed heat source as a superposition of a large number of point heat sources that have power levels giving a Gaussian distribution. In principle, this approach can be used for any distribution in the x, y and z planes.

Eagar and Tsai [48] used Green’s functions to find a solution for an arbitrary distributed heat source ($Q^*$) in a moving coordinate systems, as shown in Eq 4.13.

\[
\frac{\partial^2 \theta^*}{\partial w^2} + \frac{\partial^2 \theta^*}{\partial y^2} + \frac{\partial^2 \theta^*}{\partial z^2} - \left( \frac{\nu}{2\kappa} \right)^2 \theta^* = -e^{\frac{vw}{2\kappa}} \frac{Q^*}{\lambda} \tag{4.13}
\]

In this case;

\[
\theta^* = (\theta - \theta_0)e^{\frac{vw}{2\kappa}} \tag{4.14}
\]

where $Q^*$ is the moving heat source. It is important to note that the notations are similar to those used in Section 4.1.1.

While this approach is valid, the general solution to this equation is difficult to find. In order to simplify the problem, it is possible to represent the heat source by many small heat sources (differentiate the heat source) with the appropriate values. For example, if
\[ \delta Q \text{ is the amount of heat generated at location defined at a position (x',y',z') at a given time (t'), the change in temperature } (d\theta_t) \text{ at that time is defined as:} \]

\[
d\theta_t = \frac{\delta Q dt'}{\rho c(4\pi\kappa(t - t'))^{\frac{3}{2}}} e^{-\frac{(x-x')^2 + (y-y')^2 + (z-z')^2}{4\alpha(t-t')}} \tag{4.15} \]

By substituting the equation for a Gaussian heat source, Q, [Eq. 4.14] into [Eq. 4.14] and integrating over the entire area (adding all the small \(\delta Q\)), the change in temperature then becomes:

\[
d\theta_t = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{q}{2\pi\sigma^2} e^{-\frac{(x-x')^2}{2\sigma^2}} \frac{dt'}{\rho c(4\pi\kappa(t - t'))^{\frac{3}{2}}} e^{-\frac{(x-x')^2 + (y-y')^2 + (z-z')^2}{4\alpha(t-t')}} dx' dy' \tag{4.16} \]

This equation describes the change in temperature at any location in a semi-infinite (see Figure 4.2) body with a Gaussian type heat source. In order to consider the situation where the heat source is traveling, it is possible to integrate Eq 2.17 over a given weld time (t'). In more detail, Eq. 4.17 describes the heat input for a single heat source for a given time (t') and location (x',y',z'). Since the required model has a moving heat source, all that is required is to add (integrate) the effects of the heat source from time (t=0) to a particular time (t) of interest;
\[\theta - \theta_0 = \frac{q}{\pi \rho \chi (4\pi \kappa)} \int_{0}^{t} \frac{(t - t')^{\frac{3}{2}}}{2\kappa (t - t') + \sigma^2} \exp\left(-\frac{(x - vt')^2 + y^2}{4\alpha(t - t') + 2\sigma^2}\right) - \frac{z^2}{4\kappa(t - t')} dt' \] \ [4.17]

It is important to note that in this case, it is simpler to use a moving coordinate system as detailed in Section 4.1.1. While Eq. 4.17 can be solved numerically, it is possible to further simplify the model by substituting a dummy variable time \((t'')\) that is defined as \(t'' = t - t'\). That is to say \(t''\) is simply the time when the heat source is at a location of interest. By making this definition, several other relationships can be determined:

\[\frac{dt''}{dt'} = -v\]

\[x - vt' = w + vt''\] \ [4.18]

By substituting these definitions into Eq 4.18, one gets:

\[\theta - \theta_0 = \int_{0}^{t} \frac{q}{\pi \rho \chi (4\pi \kappa)} t''^{-\frac{3}{2}} \exp\left(-\frac{w^2 + y^2 + 2wvt'' + v^2 t''^2}{4\alpha t'' + 2\sigma^2}\right) - \frac{z^2}{4\kappa t''} dt'' \] \ [4.19]

Again, this equation must be solved numerically, but in this case, all the variables are defined in terms of the moving coordinate system.
4.1.3 SQUEEZE FLOW OF ASPERITY PEAKS

When two polymer interfaces (faying surfaces) are brought together, there are microscopic peaks and valleys (asperity peaks), see Figure 4.6(a). The number and size of these asperity peaks depend on the material and processing of the substrate. During welding, these asperity peaks are softened and flow so as to fill the interstitial spaces, see Figure 4.6 (b).

![Figure 4.6 Cartoon of polymer interface with asperity peaks, (a) before welding and (b) after welding](image)

In order to better understand this flow, it is proposed that the surface can be modeled as many small, identical cylinders of material placed between two rigid plates separated by some arbitrary distance $2h$. In addition, in order to simplify the model, only a single asperity will be modeled, see Figure 4.7.
In this model, the original height and radius is defined as $h_0$ and $r_0$, respectively. The final radius is defined as $r_{\text{od}}$. By making the following assumptions:

1. Newtonian fluid properties of the melt
2. Constant material properties ($\frac{\partial \rho}{\partial t} = 0$, where $\rho$ is material density)
3. Fully developed flow
4. No slip condition at interfaces ($z=h$ and $z=-h$)
5. Symmetry ($\frac{\partial}{\partial \phi} = 0$)
6. The flow path is much greater than the gap ($r>>2h$)
7. No body forces (B) such as gravity
8. Lubrication approximation
9. No inertial effects

The Navier-Stokes Equations, Eq 4.20 and continuity equation, Eq. 4.21, in cylindrical coordinates can be used to approximate the flow;

r-axis;

\[
\rho \left( \frac{\partial v_r}{\partial t} + v_r \frac{\partial v_r}{\partial r} + \frac{v_\phi}{r} \frac{\partial v_r}{\partial \phi} + \frac{v_z}{r} \frac{\partial v_r}{\partial z} \right) = - \frac{\partial P}{\partial r} + \mu \left[ \frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial (r v_r)}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v_r}{\partial \phi^2} - \frac{2}{r^2} \frac{\partial v_\phi}{\partial \phi} + \frac{\partial^2 v_r}{\partial z^2} \right] + B_r
\]

z-axis

\[
\rho \left( \frac{\partial v_z}{\partial t} + v_r \frac{\partial v_z}{\partial r} + \frac{v_\phi}{r} \frac{\partial v_z}{\partial \phi} + v_z \frac{\partial v_z}{\partial z} \right) = - \frac{\partial P}{\partial r} + \mu \left[ \frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial v_z}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v_z}{\partial \phi^2} + \frac{\partial^2 v_z}{\partial z^2} \right] + B_z
\]

Where, \( \nu \) is flow velocity and \( \mu \) is viscosity. The \( \phi \)-axis is not considered because of symmetry assumption made (assumption number 5). Based on assumptions #2 and #5, the continuity equation reduces to Eq 4.22.
Because the two final portions of the continuity equation sum to zero and are only a function of r and z, respectively, they must also be equal to zero, that is to say \( F(r) = G(z) = 0 \). Thus, it is possible to reduce the flow in the r-direction to Eq 2.23.

\[
\rho \left( \frac{\partial v_r}{\partial t} + v_r \frac{\partial v_r}{\partial r} + \frac{v_\phi}{r} \frac{\partial v_r}{\partial \phi} + \frac{v_z^2}{r^2} \frac{\partial v_r}{\partial \phi} \right) = -\frac{\partial P}{\partial r} + \mu \left[ \frac{\partial}{\partial r} \left( \frac{1}{r^2} \frac{\partial (rv_r)}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v_r}{\partial \phi^2} - \frac{2}{r^2} \frac{\partial v_\phi}{\partial \phi} \right] + \frac{B_s r^2}{\mu} \tag{4.23}
\]

\[
\therefore \frac{\partial P}{\partial r} = \mu \frac{\partial^2 v_r}{\partial z^2}
\]

By integrating Eq 4.23 with respect to z, and using the boundary conditions to solve for the integration constants;

\[
z = 0 \text{ the velocity profile is zero } \left( \frac{\partial v_r}{\partial z} = 0 \right) \text{ (Stagnation point)}
\]
z=h, -h, velocity is zero (ν=0) (Assumption #4)

it is possible to define the flow velocity in the r direction as seen in Eq 4.24.

\[ \nu_r = \frac{1}{2\mu} \frac{\partial p}{\partial r} (z^2 - h^2) \]  [4.24]

By substituting Eq 4.24 into Eq. 4.23 and integrating over the volume (h and r) as seen in Eq. 4.25, and setting \( \nu_z = \frac{dh}{dt} \) at \( y=h, -h \),

\[ \int_0^h \int_0^r \frac{1}{r} \frac{\partial}{\partial r} \left( \rho r \frac{1}{2\mu} \frac{\partial p}{\partial r} (z^2 - h^2) \right) drdz + \int_0^h \int_0^r \frac{\partial}{\partial z} (\rho \nu_z) drdz = 0 \]  [4.25]

it is possible to define the pressure gradient in the r-direction (\( \frac{\partial p}{\partial r} \)) as seen in Eq 4.26.

\[ \frac{\partial p}{\partial r} = \frac{3r\mu}{2h^3} \frac{\partial h}{\partial t} \]  [4.26]

Integrating Eq. 4.26 over r, and setting p=0 at \( r=r_{od} \) (no pressure at edge of melt), the pressure (P) as a function of r can be defined as seen in Eq 4.27.

\[ p = \frac{3r\mu}{4h^3} \frac{\partial h}{\partial t} \left( r^2 - r_{od}^2 \right) \]  [4.27]
In order to find the force (F) required to close the gap, h, it is possible to integrate Eq 4.27 over the contact area of the melt, from \( r=0 \) to \( r_{od} \) and \( \phi=0 \) to \( 2\pi \).

\[
F = \int_{0}^{2\pi r_{od}} \int_{0}^{r} r \frac{3\mu \partial h}{4h^3} (r^2 - r_{od}^2) \, dr \, d\phi = \frac{3\mu r_{od}^4}{8h^3} \frac{\partial h}{\partial t} \tag{4.28}
\]

By conservation of mass, it is possible to define the time varying radius (\( r_{od} \)) as;

\[
r_{od} = \sqrt{\frac{r_0^2 h_0}{h}} \tag{4.29}
\]

By substituting Eq 4.29 into Eq 4.28 and using separation of variables it is possible to define the non-dimensional relationship of \( h_0/h \);
\[
\frac{\partial h}{\partial t} = \frac{4Fh^5}{3\mu r_0^4h_0^2} \Rightarrow \int_0^t \frac{4Fh^5}{3\mu r_0^4} dt = \int_{h_0}^h h_0^2h^{-5} dh
\]

\[= \frac{4F}{3\mu r_0^4} t = \frac{h_0^2 h^{-4}}{-4} \bigg|_{h_0}^h = \frac{1}{4} (h_0^{-2} + h_0^2 h^{-4})
\]

\[= \frac{4F}{3\mu r_0^4} t = \frac{1}{4} \left(1 + \frac{h^4}{h_0^{-4}}\right) \Rightarrow \frac{16Fh_0^2}{3\mu r_0^4} t = \left(1 + \frac{h_0^4}{h^4}\right) \tag{4.30}
\]

\[
\frac{h_0}{h} = \left[\frac{16Fh_0^2}{3\mu r_0^4} t - 1\right]^{1/4}
\]

Eq. 4.30 can then be used to predict the gap height as a function of time, or more importantly the closing of two faying surfaces as function of time.

**4.1.4 MOLECULAR HEALING**

As the faying surfaces come into intimate contact, healing of the interfaces occurs. It is important to note that, even before the squeeze flow has brought the entire faying surfaces in contact, healing of interfacial regions initiates where the contact is made. Healing of the interfaces is basically diffusion of polymer chains across the interface from one side to the other. This mechanism is depicted in Figure 4.8 at various times and degrees of healing. At complete healing, polymer chains from each side of the
interface migrate across the interface so that it essentially becomes indistinguishable from the bulk material.

![Diagram](image)

Figure 4.8 Details molecular diffusion and interfacial healing

The time required to achieve full healing is primarily determined by the molecular structure of the polymer, including its molecular weight, chemical structure, and time and temperature. Other factors, such as pressure, can also affect this process. The diffusion of polymer chains can be modeled using the reptation theory proposed by DeGennes [49, 50]. In this model, each polymer chain is considered to be contained in an imaginary tube of length L. This imaginary tube is defined by constraints of neighboring polymer chains and thus, the ends of the polymer chains have more mobility compared to the bulk of the chain. The distance that a chain travels outside the original tube is referred to as the
diffusion distance $<l>^2$, and it can be related to time as shown in Figure 4.9. In this case, the diffusion distance is noted as “$<l>$” is the mean square distance.

$<l>^2 = 2D_t t$

Figure 4.9 Details of molecular diffusion and interfacial healing and Einstein’s diffusion equation

It is possible to relate the mean diffusion distance squared ($<l>^2$) of any one chain near the interface to the distance that chain propagates across the interface ($X$) as shown in Eq. 4.31 [51].

$$X \approx \sqrt{<l>^2}$$ [4.31]
By using Einstein’s diffusion equation and Eq. 4.31, where D is the diffusion coefficient, it is possible to show that healing time is related to time by a power of 1/4, as shown in Eq. 4.32.

\[
\langle l \rangle^2 = 2Dt \Rightarrow l = \sqrt{2Dt} \Rightarrow X = (2Dt)^{\frac{1}{4}}
\]

\[
\therefore X \sim t^4
\]

[4.32]

In addition, Jud [52] proposed that the diffusion coefficient is an arrhenius function of temperature (T) and it can be expressed as shown in Eq 4.33.

\[
D(T) = D_0 e^{\left[\frac{-E_a}{RT}\right]}
\]

[4.33]

where \(D_0\) is the diffusion constant, \(E_a\) is the activation energy and \(k\) is the Boltzmann constant \((1.3807 \times 10^{-23} \text{ J/K})\). While many investigators have assumed that activation energy is temperature-independent, there is data in the open literature that suggest differently. For example, Loos and Dara [53] studied the healing of polysulphone and assumed an activation energy to be temperature-independent. Loos plotted the degree of healing (autohesion) as a function of \(t^{1/4}\) for various temperatures. In this case, the
degree of healing (Dh) is defined as a ratio of degree of healing to full healing (bulk material strength) represented in terms of strength, as shown in Figure 4.10.

By plotting the natural logs of the slopes of the various temperatures of Figure 4.10 as a function of the reciprocal of the temperature, it is possible to estimate the activation energy by evaluating the slope of this relationship, see Figure 4.11. In this figure, the solid line is the slope assumed by Loos. While this estimate is reasonable, it is proposed, that a better fit is one that has a slope that is temperature-dependent (dashed line).

Figure 4.10 Degree of healing as a function of time for polysulphone [53]
In this case, it is again proposed that the relationship between the activation energy and temperature follows an exponential form:

\[ E_a (T) = A_0 e^{-k_a T} \]  

[4.34]

where \( A_0 \) is a material constant (units of J) and \( k_a \) is the temperature parameter (1/K). From Loos’s data, in this case \( A_0 = -1.72 \times 10^{-3} \) (J) and \( k_a = 3300 \) (1/K) the activation energy is plotted in Figure 4.12 as a function of temperature.
In addition, Wool [54] studied polystyrene and similar trends are also seen. While a relatively narrow range of temperatures (9°C) and number of temperatures (3 levels) were studied, again it is seen that activation energy is temperature-dependent (Figure 4.13).

Figure 4.12 Activation energy/k as a function of temperature for polysulphone
Figure 4.13 Plot of activation energy as a function for temperature for PS as report by Wool

4.1.5 COMBINED SQUEEZE FLOW AND INTERMOLECULAR DIFFUSION MODEL

In section 4.1.3 and 4.1.4, the squeeze flow of asperity peaks and molecular healing are both defined to be proportional to the forth root of time. Because both processes (squeeze flow and healing) occur during welding and follow similar trends, it is proposed that both processes can be lumped into a single expression. Because most industrial welding processes produce temperature histories that are time-dependent, it is possible to

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simplify the temperature histories by dividing a given temperature history into finite time intervals \((\Delta t)\). In this case, assuming no healing prior to welding, and assuming welding occurs between time \(=0\) and \(t'\), it is proposed that the degree of healing and squeeze flow (DW) can be defined as:

\[
DW(T, t) = \sum_{t=0}^{t=t'} K_0 \cdot e^{-\frac{E_a(T)}{RT}} \cdot \Delta t^{\frac{1}{4}},
\]

where \(A_0\), \(k_a\) and \(K_0\) can be determined experimentally and represent both squeeze flow and healing processes.

\[4.35\]

4.1.6 LITERATURE REVIEW

In previous studies, heat flow models were used to predict weld size for laser microwelding [55]. As with any modeling, there were a number of assumptions made for simplification reason. One of the assumptions that is questioned and refined in this work is that welding/healing occurs at a critical, time-independent temperature. That is to say, it is proposed here that better model predictions can be made by evaluating time and temperature effect on molecular healing.
The widths of the welds were estimated by evaluating the temperature distribution and by determining the location in the y-direction at which the peak temperature exceeded the melt temperature (processing temperatures) of the materials. The processing temperatures were determined by initially evaluating the range of processing temperature used for each material. Then, the weld width predictions were compared to the experimental values at various temperatures. A temperature was then selected by minimizing the error between the experimental and the predicted values. For PS, the processing temperature was 150°C and for PC the processing temperature was 260°C.

The initial model (point heat source) has the advantage that it is relatively simple, but it is limited, because it does not accurately represent the power distribution of a laser, which has a Gaussian distribution. Despite this initial concern with this model, it was compared to the distributed model in order to determine the degree of its accuracy. Because the distributed heat source model should provide more accurate results, it was evaluated first in order to form a base line for comparison.

Figure 4.14 shows the weld width as a function of travel speed for the distributed model at various power levels as well as the experimental values. It is seen that the model under-predicts weld widths at higher power levels, 167 mW, and over-predicts at the lower power level, 46 mW. It is proposed that this error is caused by the model’s single temperature assumption. At the higher power level, the welds have a higher heat input and thus experience longer time/temperature histories. Thus, at the higher power levels, a
point outside the predicted weld width experiences a thermal history near the critical weld temperature for a time period long enough to promote healing. Because the model does not account for this effect, it under-predicts the weld width. At the lower power levels, the time/temperature history is shorter and even though a particular point in the weld may have achieved the critical temperature, its time at this temperature was too short to allow healing. Thus, in this case the model over-predicts the weld width.

Figure 4.14 Weld width as a function of travel speed; experimental and predicted values (25 μm lens with PS)

As stated previously, the weld width predictions were based on a single processing temperature for each material. However, since welding is a molecular diffusion process, which is time- and temperature-dependent, there is probably a temperature range that correlates to the predicted weld width. Wool [56] has reported that adhesion (welding)
between two PS interfaces can occur at temperature as low as 120°C over a period of about 10 seconds. Thus, this was considered the lower value that welding when welding could occur. The upper value was considered to be 225°C (upper injection molding temperature for PS). With these assumptions, it is possible to plot the weld width as a function of travel speed with a window of predicted values, see Figure 4.15. The graph only shows one power level (107 mW) in order to reduce confusion. It is seen that if a processing temperature range in considered, the experimental values fall within the predicted values. It is also seen that the point heat source model predicts weld width as accurately as the distributed heat source model. Over this narrow range of small values of the dimensionless distribution parameter ($\mu=0.74$ to 1.45) the two models predict nearly the same weld width values.

![Figure 4.15](image.png)

Figure 4.15 Experimental data and predicted weld width for both point heat source and distributed models as a function of travel speed (25 μm lens with PS, 107 mW)
Figure 4.16 shows a similar graph for the power levels of 47 and 167 mW where only the point heat source model is plotted. It is seen that nearly all the experimental data falls within the predicted weld width range (temperature range). However, it is again seen that at higher power levels the model typically under-predicts the weld width.

Figure 4.16 Experimental and predicted weld width for point heat source model as a function of travel speed (25 μm lens with PS)
Figure 4.17 compares the predicted weld width as a function of power for PC. Again, it is seen that at higher power levels the model typically under-predicts weld width.

In short, while this study allowed reasonable prediction of weld widths based on a single temperature. The overall approach relied on finding a single critical healing/welding temperature that was a compromise in order to make reasonable weld width predictions. Better model predictions were made by defining a temperature range, but this reduced the accuracy of the model.
4.2 EXPERIMENTAL PROCEDURES FOR MOLECULAR HEALING

4.2.1 MATERIALS AND SAMPLES

Two thermoplastic materials were used in this study, polycarbonate (PC) and polystyrene (PS). They were selected because they represent materials that will probably be used in the MEMS industry. Tables 2.1 and 2.2 provide details of mechanical and thermal properties for these materials.

In order to determine molecular healing coefficients, welds were made with a reinforced lap shear configuration for both PC (180 μm thick) and PS (80 μm thick). A 40 μm thick Kapton adhesive tape was applied to the external surfaces of the lap shear joint in order to ensure that failure occurred in the weld and not in the bulk sample. The overlap of the joint was held constant between 750 and 900 μm. This overlap was manually adjusted and held constant during welding with Kapton tape at the edges of the weld which was discarded after welding. The final overlap measured and recorded. This joint geometry was selected because it ensured that failure occurred at the faying surfaces.
In order to further ensure that failure occurred at the faying surfaces, prior to mechanical testing, 5 mm’s of each edge of the sample was removed to eliminate edge effects. In addition, a semi-circle pattern was cut from the final edges of the sample centered on the weld line. These modifications (preparations) to the weld samples are shown in Figure 4.19.
For weld width models verification, welds were made on 25.4 mm x 25.4 mm samples, as shown in Figure 4.20.
4.2.2 WELDING FOR MOLECULAR HEALING

4.2.2.1 IMPULSE WELDING FOR MOLECULAR HEALING MEASUREMENTS

In initial studies, a commercially available dual-sided heating impulse welding system was used (an American International Electric AIE 350FD model). However, the cooling time (+4 s) was considered too long in order to produce temperature histories representative of micro-laser welding (50-500 ms). Additional studies were completed with the same system, except that once the heating cycle was completed, the electrodes were quickly opened so the weld could be chilled with compressed air. While this
reduced the cooling time, it resulted in warpage and deformation of the weld that prevented proper mechanical testing of the weld samples.

Because of the difficulties encountered with the commercially available impulse welding system, a customized impulse welding system was designed and constructed. The design was based on water cooling of the welding heads immediately after the heating cycle was completed. The water cooling channels were placed as near to the heating element (0.050” (1.3 mm)) as possible, while still maintaining structural integrity of the welding head. Similar to the commercial impulse welding system, heating from both sides (top and bottom) was used to reduce heating times. The heating element was a 5 mm wide nichrome band. Kapton tape was used as a release agent between the heating elements and samples. The overall design of one head is shown in Figure 4.21. It is seen that springs (tension springs) are added to ensure that the heating element is maintained under tension despite thermal expansion during weld.
A constant current DC power supply (Xantrex XFR-40-70, max. current; 40 amp, max. voltage; 70 V) was used to supply electrical power to the heating elements. The upper and lower electrodes were attached in series. A Polyscience Recirculator 340 water chiller was used to regulate water flow. Relay timers, solenoid and remote control inputs on the DC power supply were used to control the system. Figure 4.22 shows the control system for the impulse welding system.
In order to account for the slight delay in cooling of the joint interface due to thermal conduction through the welding head, heating element and release agent (Kaptone tape), the water cooling was solenoid was activated 0.5 s before the heating current was discontinued.
A 36 gauge K-type thermocouple was placed at the weld interface of a sacrificial sample to measure the temperature during welding. The temperature was recorded with a PC-based data acquisition system with a sampling rate of 50 Hz.

4.2.2.2 SCAN WELDING

The laser system used in this study was a Coherent F-system. The system is based on a single laser diode that is fiber-coupled to a focusing lens. The fiber was relatively flexible with a diameter of 50 μm and was approximately 50 cm long. This allowed the laser to be delivered remotely. The specifications of the laser system are shown in Table 4.1.
<table>
<thead>
<tr>
<th>Characteristic</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak wave length</td>
<td>828.5 nm</td>
</tr>
<tr>
<td>Maximum power</td>
<td>850 mW</td>
</tr>
<tr>
<td>Fiber optic cable</td>
<td>50 μm dia.</td>
</tr>
</tbody>
</table>

Table 4.1 Specification of laser welding system

Two focusing lenses manufactured by Coherent were used, see Table 3.5. They were standard spherical lenses with a specially manufactured housing, which was also supplied by Coherent.

<table>
<thead>
<tr>
<th>Lens</th>
<th>Specified focal spot dia.</th>
<th>Specified focal length</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>25 μm</td>
<td>14 mm</td>
</tr>
<tr>
<td>50</td>
<td>50 μm</td>
<td>28 mm</td>
</tr>
</tbody>
</table>

Table 4.2 Specifications of focusing lenses

The focal distance was confirmed by measuring the resulting weld width at constant welding parameters (see Table 3.6) and at various distances. The distance was measured from the front of the black mounting ring of the lens to the top surface of the black sample.
### Table 4.3 Measured focal distance calibration for each lens

<table>
<thead>
<tr>
<th>Lens</th>
<th>Setting</th>
</tr>
</thead>
<tbody>
<tr>
<td>25 μm</td>
<td>15.5 to 15.7 mm</td>
</tr>
<tr>
<td>50 μm</td>
<td>28.0 to 28.5 mm</td>
</tr>
</tbody>
</table>

Because previous investigations [57] have shown that very small gaps or voids at the interface can prevent welding with a scan welding method, uniform weld pressure was applied by using a transparent pressure bladder [58]. The basic concept is that the transparent bladder is relatively flexible so that once it is inflated, it presses the clear film of the sample and applies a weld pressure (see Figure 4.24). The laser passes through the PC window, the transparent bladder, and the top film to heat the interface.

![Figure 4.24 Cross-section of welding fixture with bladder on top](image-url)
In order to measure the power delivered to the weld, a thermopile power meter (Coherent Lab-Master) was used to measure the power at various power settings (0 to 1,000 mA) with the laser beam passing through the same materials and interfaces used in an actual welding setup.

The heat input \( (q, \text{ J/mm}) \) to the sample was calculated using Eq. 4.36.

\[
q = \frac{P_w}{v} \quad \text{[4.36]}
\]

Where \( P_w \) (W, J/s) is the power at the weld and \( v \) (mm/s) is travel speed.

In initial trials, a standard DC-motor-driven table was used to translate the parts relative to the laser source. However, due to problems with fluctuations in the travel speed, which resulted in fluctuations in weld quality, a stepper motor was used in later tests. The speed was monitored using an LVDT and PC-based data acquisition system. The stepper motor was manufactured by Applied Motion Products (200 S/R) and was controlled by a PC. The interface software was also provided by Applied Motion Products (NMCTest). The slide table was manufactured by Parker (105022P-10E) and had approximately 50 mm of travel. While the system had a maximum stable travel speed of 100 mm/s, it could travel as fast as 120 mm/s but often became unstable at speeds above 100 mm/s. Unstable behavior was noted as fluctuation in the travel speed. The motor drive setting (0 to 380) in the software was correlated to travel speed using the
LVDT and PC-based data acquisition system. Figure 4.25 shows a photograph of the entire weld system.

Figure 4.25 Photograph of weld system

In order to gain an understanding of the welding process, three primary experiments were conducted:

1) Melt (no welding) width (for PC and PP) as a function of travel speed and power
2) Weld width (for PC and PS) as a function of travel speed and power
3) Weld strength (for PC only) as a function of travel speed, weld pressure and power.

The range of parameters that were studied is shown in Table 4.6.
Table 4.6 Summary of parameters and ranges that were studied

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Term</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power</td>
<td>$P$</td>
<td>20 to 600 mW (at the weld surface)</td>
</tr>
<tr>
<td>Travel speed</td>
<td>$V$</td>
<td>5 to 60 mm/s</td>
</tr>
<tr>
<td>Pressure</td>
<td>$Pr$</td>
<td>0.05 to 0.5 MPa</td>
</tr>
</tbody>
</table>

4.2.3 MOLECULAR DIFFUSION DESIGN OF EXPERIMENTS

For clarification, there were six major task/experiments conducted in this section for the two materials studied. These tasks are detailed in Figure 4.26.
4.3 RESULTS AND DISCUSSION FOR MOLECULAR HEALING

4.3.1 MOLECULAR DIFFUSION EXPERIMENTS WITH PS

The initial experiments in this section evaluated weld strength as a function of time at relatively low temperatures and long weld times. This data was then used to determine
the activation energy as a function of temperature. Figure 4.27 shows the measured
temperature at the bondline during a 100 s weld cycle. For reference, the desired
temperature profile is also plotted where the temperature instantaneously heats and cools
to and from the desired weld temperature (86°C). It is seen that, while there is some
deviation from the desired temperature profile, there is reasonable agreement.

![Temperature profile graph](image)

**Figure 4.27** Measured and ideal temperature profile for long-term heating/welding

In more detail, Figure 4.28, shows weld strength as a function of weld time raised to \( \frac{1}{4} \)-power. With PS, the maximum weld strength was measured to be 4 N/mm and thus this stress was taken as the strength of a fully healed interface. As expected, the relationship between strength and time^{\frac{1}{2}} is linear (Eq. 2.34). Thus, with each temperature plot there is a corresponding linear fit (least square method) with the intercept defined as zero. Each
relationship (the slope) can then be used to calculate the time \((t_\infty)\) required to achieve full healing at each temperature. In these experiments, the maximum weld strength reported was approximately 4 N/mm and thus was assumed to be the strength corresponding to complete healing. As expected, the time required to achieve complete healing is inversely proportional to temperature. That is to say, it is seen that at 90°C, the time required to achieve full healing is 1183 s, while at 142°C, the time is only 6.38 s.

![Graph showing weld strength as a function of time for various temperatures.](image)

Figure 4.28 Weld strength as a function of time^{1/4} for PS at various temperatures
By taking the ratios of Eq 2.36 for two separate temperatures, it is possible to calculate the activation energy based on a common degree of healing. For example, with a defined level of 100% healing, the activation (energy/R) can be calculated using Eq 4.33 based on two temperatures, T1 and T2. In this case, t1 and t2 are the times required to achieve full healing for T1 and T2 respectively.

\[
\frac{E_{T_{\text{avg}}}}{R} = \frac{\ln\left(\frac{t_{1\infty}}{t_{2\infty}}\right)}{\left(\frac{1}{T1} - \frac{1}{T2}\right)}
\]

[4.37]

In this case, the activation energy/R is based on the average temperature (T_{\text{avg}}) for T1 and T2. It is important to note that with four temperatures, there are six possible combinations that can be used to calculate the activation energy. Each combination resulting in a unique average temperature. Thus, based on the data in Figure 4.28 (four different temperatures) it is possible to calculate a total of six activation energies. Based on this approach, Figure 4.29 shows the activation energy/R as a function of temperature. It is important to note that in this case, the activation includes Boltzmann’s constant. As expected, the activation energy is inversely proportional to temperature.
By assuming the form proposed in Eq. 2.34, and by plotting the natural log of the activation energy/R as a function of temperature, Figure 4.30, it is possible to use a least squared fit method to determine the coefficients proposed in Eq. 2.36. In this case, the linear fit to the line is \( \ln \left( \frac{E_a}{k(T)} \right) = 21.079 - 0.0254T \).
Thus, the activation energy/R as a function of temperature is:

$$E_a(T) = 1.427 \times 10^9 e^{-0.0254*T}$$

[4.38]

This equation is also plotted in Figure 4.29 and it is seen that there is good agreement with the experimentally determined values.
The temperature profiles made with the short cycle times (<4 s) were relatively dynamic compared to the profiles shown in Figure 4.27. That is to say that with the short cycle times, the heating and cooling portions of the temperature cycle was a significant amount of the entire temperature history. This is seen Figure 4.31, which shows selected temperature profiles for various power levels (25-35 amps) and cycle times (1.6-3.5 s). It is seen that despite the current level, the heating rate is relatively constant. However, the steady state temperature for various power settings is different. For example, with a power setting of 40 amps (1.47x10^6 W/m^2) the steady state temperature is approximately 440 K, while at 25 amps (0.52x10^6 W/m^2) the steady temperature is 385 K. It is also seen that in some of the settings, such as that seen at 35 amps (1.06x10^6 W/m^2), the cycle time was too short (1.6 s) to allow the system to reach steady state. Thus, it is impossible to assume a particular welding/healing temperature and the heating a cooling portion of the profile is the most critical portion of the temperature history.
Figure 4.31 Typical temperature profiles for short cycle times for selected heating cycles

Figure 4.32 shows weld strength as a function of weld time at various current setting. It is seen that weld strength is proportional to weld time and current as expected. In addition it is seen that with extended weld times, the weld strength tends to drop off as a result of over-welding and film damage. This was evident by visual inspection of the welds were excess squeeze flow could be seen. It is also seen that maximum achievable weld strength is approximately 4 N/m, which was taken as the value for 100% healing.
By evaluating all the welding parameters (power settings and cycle times), the final parameter \( K_0 \) in Eq. 2.37 can be iteratively determined. In this case, it was found that it was \( 0.04 \, \text{s}^{-\frac{1}{2}} \). Using the developed model and temperature histories, the degree of healing was calculated for the various short time impulse welds. In Figure 4.33, the experimental degree of healing is plotted as filled points, and the model is plotted as unfilled points. In addition the arrows represent the difference between the predicted and experimental values. It is seen that the model is in relatively good agreement with the experimental values.
Figure 4.33 Experimental and model degree of healing as function of weld time at various current settings for impulse (PS)

Figure 4.34 shows a plot of the predicted healing value and actual healing value for all welding conditions. Ideally, all the data would fall on a 45° straight line with a one-to-one correlation. While it is seen that at the lower values (10% healing) the model slightly over-predict the values, the model does a reasonably job of predicting the degree of healing.
4.3.2 MOLECULAR DIFFUSION EXPERIMENTS WITH PC

Figure 4.35 shows weld strength as a function of weld time raised to $\frac{1}{4}$-power for PC. With PC, the maximum weld strength was measured to be 11 N/mm and thus this stress was taken as the strength of a fully healed interface. As expected, the relationship between strength and time $t^{\frac{1}{2}}$ is linear (Eq. 2.34). Thus, with each temperature plot there is a corresponding linear fit (least square method) with the intercept defined as zero. Each relationship (the slope) can then be used to calculate the time ($t_\infty$) required to achieve full healing at each temperature, which is detailed in the figure.
By assuming a form proposed in Eq. 2.36, and by plotting the natural log of the activation energy/k as a function of temperature, it is possible to use a least squared fit method to determine the coefficients proposed in Eq. 2.36. In this case, the linear fit to the line is

$$\ln \left[ \frac{E_a}{k(T)} \right] = 23.39 - 0.0378T.$$
Figure 4.36 Activation energy as a function of temperature for PC

Figure 4.37 shows weld strength as a function of weld time at various current setting for PC. It is seen that weld strength is proportional to weld time and current as expected. In addition, it is seen that with extended weld times, the weld strength tends to drop off as a result of over-welding and film damage. It is also seen that the maximum achievable weld strength is approximately 11 N/m, which was taken as the value for 100% healing.
Figure 4.37 Weld strength as function of weld time at various current settings for impulse welds with PC (Polynomial fitted lines added for visual reasons)

By evaluating all the welding parameters (power settings and cycle times), the final parameter (K₀) in Eq. 2.37 can be iteratively determined. In this case, it was found that it was 0.55 s⁻¹. Using the developed model and temperature histories, the degree of healing was calculated for the various short time impulse welds. In Figure 4.38, the experimental degree of healing is plotted as filled points, and the model is plotted as unfilled points. In addition the arrows represent the difference between the predicted and experimental values. It is seen that the model is in relatively good agreement with the experimental values.
This verification of the model was based on comparison of experimental weld widths and predicted weld widths. In this case, the welds were made using a scanning technique as detailed in Section 4.2.2. Because the welds were relatively small (<200 μm in width), it was not practical to use thermocouples to measure the bondline temperature. Thus, temperature fields were predicted using the models detailed in Section 4.1.1 and 4.1.2. For those welds made with the lens noted as 25 μm, the point heat source model (Section 4.1.1) was used. This choice was made based on previous findings that this model was
sufficient to predict temperature fields with this welding configuration [55]. For those welds made with the 50 μm lens, the distributed heat source model (Section 4.1.2) was used.

Weld widths were determined by predicting the temperature history at the faying surface (z=0 m) at various y-distances from the weld center line. This temperature history was then used to calculate the degree of healing based on Eq 2.35 and those parameters defined in Section 4.5.

Before this model is reviewed, the value of K₀ must be reviewed in some detail. As noted in the experimental section, the experimental data was recorded at a sampling rate of 50 Hz. This rate was selected because it was the upper response rate of the thermocouples. However, during the modeling of microwelds, the time interval was set to 1/50,000 s in order to assure sufficient data points are collected during the relatively short temperature histories. Because the product of (K₀ · Δt¼) for both sampling rates should be equal, a new value of K₀ is needed for the smaller time interval (Δt). In this case the new value for K₀ should be approximately 0.0070 s¼. However, in order to increase the accuracy of the K₀ it was redefined to 0.175s¼. The difference between the expected and actual values is most likely due to difference in material composition of the different grades of PS used between the impulse and scan microwelding experiments.
Various distances were evaluated in an iterative process until a degree of healing of approximately 100% was predicted. This distance was then multiplied by 2 in order to estimate the weld width.

In order to confirm that a 100% degree of healing corresponds the degree of healing at the edge of weld for weld widths predictions, a sensitivity study was completed on the degree of healing. That is to say, weld widths were modeled using four levels of healing (0, 0.25, 0.5, 0.75 and 1.0). Figure 4.39, shows a plot of weld widths as a function travel speed for 167 mW. Again the points correspond to the experimental data and the lines correspond to the various model predictions at various degrees of healing. It is seen that the various levels do responsibly well in predicting weld width. Comparing the $r^2$ factor for all three values, they all fall between 0.995 and 0.996. It is seen there is little difference between any of the degree’s of healing.
Figure 4.39 Weld width prediction as a function of travel speed for various degree of healing

To further illustrate the difference in the predicted weld width as a function of the degree of welding, Figure 4.42 shows the predicted degree of healing as a function of distance from the weld center line. In the figure, a picture of a small section of a micrograph of a microweld is superimposed on the graph to add in visualization. It is seen that from the weld center line and edge of the weld, the model predict a degree of healing of one (full healing). At the edge of the weld, the model predicts a degree of healing between 1 and 0, as expected. It is important to note that the degree of healing is highly independent near the edge of the weld. Thus, it is again seen that there is little difference in the final
weld width predictions based on varying degrees of healing. Thus, for consistency, a degree of healing of 1.0 was used to predicted weld widths for all models.

![Graph of Degree of Healing](image)

Figure 4.40 Degree of healing a function of distance from weld centerline (6.92 mm/s 167 mW)

Figure 4.41 shows the weld width as a function of travel speed at various power levels. It is important to note that the reported power level corresponds to the actual power at the faying surface. The dots correspond to experimental data. The dashed line corresponds to weld width predictions based strictly on a weld temperature and represent the previous methodology used to predict weld width. The thicker lines correspond to the predicted
weld widths based on thermal history and molecular diffusion. It is seen that while both methods of predicting weld width are reasonable, the technique based on thermal history is much better. That is to say, the weld width predictions based on thermal history are excellent.

Figure 4.41 Weld width as a function of speed at various power levels for various models (25 μm lens with point heat source mode)

Figure 4.42 shows a similar trend, except that in this case, only the predicted value for the thermal history model is plotted. It is important to note that in this case the welds were made with a lens noted as having a 50 μm focal spot and the temperature fields were predicted using the distributed heat source model. Again, it is seen that the model does reasonably well in predicting weld widths. The model generally under-predicted at the
higher power level (167 mW). Better results were obtained by adjusting the $K_0$ value, but this resulted in less accurate predictions for the welds made with a lens noted as 25 μm.

Figure 4.42 Weld width as a function of speed at various power levels for various models (50 μm lens with distributed heat source model)

4.3.4 MICRO WELDING MODELS WITH PC

Using the same techniques detailed in Section 4.3.1, weld width for PC were modeled. Figure 4.43 shows the weld width as a function of travel speed at various power levels for PC with the lens noted as 25 μm. Because the product of $(K_0 \cdot \Delta t^{1/4})$ for both sampling rates should be equal, a new value of $K_0$ is needed for the smaller time interval ($\Delta t$).
this case the new value for $K_0$ should be approximately $0.097 \text{s}^{1/6}$. However, in order to reduce the error between the model and experimental values, a value of $K_0=0.125$ was used. Again, the dots correspond to experimental data and the lines correspond to the predicted weld widths based on thermal history and molecular diffusion. It is seen that the model and experimental data are in very good agreement.

![Figure 4.43 Weld width as a function of power at various welding speed (25 μm lens with point heat source model)](image)

Figure 4.43 shows a similar trend, except that in this case, the welds were made with a lens noted as having a 50 μm focal spot and the temperature fields were predicted using
the distributed heat source model. Again, it is seen that the model does reasonably well in predicting weld widths. Again, the model does not predict weld width as well for the lens noted as 50 μm, compared to the lens noted as 25 μm. It is believed that better correlation can be achieved by modifying some of the constants of the healing equation. It is believed that partial defocusing of the system may be the root cause of the relatively small error between the model and the experimental data.

Figure 4.44 Weld width as a function of power at various welding speed (50 μm lens with distributed heat source model)
CHAPTER 5

MICRO-WELDING

By passing a diffractive image through a convex lens, it is possible to reduce the size of the image at a given plane, see Figure 5.1. This allows micro-features to be welded.

Figure 5.1 Diffractive optics coupled with a convex lens for image re-sizing
Because it has been proposed to use this technology for micro-welding of polymer based MEMS micro-fluidic devices, the concept must be proven. Then it is important to understand the theoretical limit of how small a weld can be made.

In practical terms, there are two major considerations that will limit the minimum achievable weld size, optical limitations and heat flow (thermal diffusion). As detailed below, the optical limitation prevents a true point heat source from being produced. Heat flow is a competing limitation that as a function of time diffuses the heat in a medium and increases the weld size. Because healing is time dependent, and there is a minimum time required to achieve a weld for a given temperature, heat flow increases the weld size. These limitations are detailed in the following sections.

5.1 OPTICAL LIMITATIONS

In this work, it is proposed to use standard optics to magnify or reduce the size of an image produced by diffractive elements. Thus, it is important to understand, that in order to produce small images, there are two physical limitations of standard convex lenses (such as a household magnifying lens), namely:

1) Diffraction limited focusing
2) Spherical aberration limited focusing
Similar to diffractive optics, a standard convex lens focuses a beam of light by superposition of light rays that are refracted (bent). At a focal plane, the superposition of the various rays results in constructive and destructive patterns. As shown in Figure 5.2, when a light ray of path CB is half a wavelength different in length than light ray path AB, a destructive (nodal) point is produced, such as seen at point B. At the focal spot, the constructive interference produces a maximum. Thus, as the distances from all the rays of light approach each other (maximum constructive interference), there is focal spot produced. As can be seen in the figure, the diameter of the focal spot depends on how fast the distances of the focal rays approach each other as a function of horizontal distance. The closer they are together, the smaller the focal spot. For example, the longer the focal length, the less the rays of light are bent allowing the diameter where the beams are in phase (same ray length) to be relatively small.

Figure 5.2 Illustration of diffraction limited focal spot
Thus, for a Gaussian beam of light, the minimum spot size \( (W_0 = \text{minimum spot diameter}) \) that contains 86% of the entire beam energy, which can be focused by a lens (limited by diffraction) is defined as [59]:

\[
W_0 = \frac{4f\lambda}{\pi D_l}
\]  

[5.1]

where \( f \) is the focal length of the lens and \( D_l \) is the lens diameter.

However, diffraction limited focusing is only one factor limiting the minimum spot size achievable with a single lens. The other limiting lens design factor is spherical aberrations. As the term implies, spherical aberrations refer to the lens geometry deviating from that of a perfect sphere. This causes rays of light that are parallel to the axis of the lens to strike the lens at various distances from the center of the lens and to be focused at various focal lengths. The end result is blurring of the focal spot. The minimum focal spot that can be formed based on spherical aberrations is [59]:

\[
W_0 = \frac{K(n, \delta, \Psi)D^3}{f^2} S_z
\]

[5.2]

In this case, \( S_z=2\Theta S_2 \), where \( S_2 \) is the distance from the lens to the image plane (ideal focal plane), \( \Theta \) is the half angle of the included beam and \( K \) is a lens geometry factor defined as:
Where $\delta$ is the lens shape factor $= (r_2+r_1)/(r_2-r_1)$, where $r_1$ and $r_2$ are the radius of curvatures of the lens faces, respectively. In addition, $\psi$ is the position factor $= 1-2f^2/S_2$ and $n$ is the index of refraction of the lens material.

Referring to Eqs 5.1 and 5.2, it is seen that for a lens with a given diameter, the minimum focal spot size is proportional to the focal length, based on diffraction limitation, and inversely proportional to focal length based on spherical aberrations. The actual minimum spot size is defined when the diffraction limited equation (Eq. 5.1) and spherical aberrations equation (Eq. 5.2) are equal. For example, Figure 5.3 shows a hypothetical focal spot size for spherical- and diffraction-limited focusing. In this case, the minimum local spot size corresponds to the intersection point of the two curves and the actual focal spot size will lay with the regions that are highlighted.
It is important to note that it is possible to use a lens system (combination of lenses) to reduce these limitations.

5.2 POINT, STATIONARY HEAT SOURCE

In order to estimate heating (temperature fields) from the smallest conceivable heat source, the heat generation can be approximated as internal heat generation in a very small sphere with a radius approaching zero (point heat source). It is further assumed
that the material properties are constant and the power is dissipated at a rate of P from time zero to \( t_w \). The model detailed in Figure 5.4 can be used to predict the temperature in a sphere with infinite radius at any point in the sphere at a distance \( r \) from the center of the sphere at any time (t) from the start of application of the heat.

**Assumptions:**
1. Constant material properties
2. \( \frac{dT}{dr}=0 \) at \( r \rightarrow \infty \)
3. Initial temp \( T \)
4. \[
    \lim_{r \rightarrow \infty} 2\pi r^2 \left(-\frac{\partial T}{\partial r} \right) = P
    \]
5. \( T=T_0+T \)

![Figure 5.4 Details of heating model of sphere](image)

It can be shown that the governing equation for heating by conduction is [60];
There is a closed-form solution for a single point heat source as a function of time and distance, as shown in Eq. 5.5 [60].

\[
\frac{\kappa}{r^2} \left[ \frac{\partial}{\partial r} \left( r^2 \frac{\partial T}{\partial r} \right) + \frac{1}{\sin \beta} \frac{\partial}{\partial \beta} \left( \sin \beta \frac{\partial T}{\partial \beta} \right) + \frac{1}{\sin^2 \beta} \frac{\partial^2 T}{\partial \phi^2} \right] = -\frac{1}{\kappa} \frac{\partial T}{\partial t}
\]

[5.4]

\[
\theta(r, t) = \frac{1}{8(\pi \kappa)^2} \int_0^t \frac{P}{C \rho} e^{\frac{-r^2}{4\kappa(t-t')}} dt'
\]

[5.5]

where \( t' \) is a dummy integration time variable.

### 5.3 THEORETICAL MINIMAL WELD SIZE

In order to gain insight to the minimum weld size possible, the healing models previously used to predict weld sizes (Eq. 2.37) were coupled with a hypothetical point heat source as detailed in Section, 5.2, namely Eq. 5.5.

In this case, the heat source is assumed to be a point heat source with a constant heating duration of \( t_w \). It is important to note that the same approach can be used for various heat sources with varying time and spatial relationship.
Before the above equation was used to predict minimum weld size, predicted temperature profiles were plotted, see Figure 5.5. In this case, the power (0.25 mW) from a hypothetical point heat source was applied for 20 ms and the temperature plotted as a function of distance (r) from the heat source. The steady state temperature profile is taken to be that depicted by the time of 20 and 2 ms because they are essentially equal. Because the temperature profiles are equal at significantly different times (a magnitude difference) then $d\theta/dt=0$ and thus steady state can be assumed. Thus it is seen that the steady state condition is reached very quickly. It is also seen that within 2 ms after the power is discontinued ($t=22$ ms) the temperature near $r=0$ already cools significantly. Thus, it can be seen that the temperature fields near the point heat are proportional to the power profile. For example, when the power is applied the temperature fields are at or near to steady state conditions, and once the power is discontinued, the temperature fields drops very quickly.

![Figure 5.5 Temperature as a function of distance from point heat source at various time (heating time=20 ms)](image)

Figure 5.5 Temperature as a function of distance from point heat source at various time (heating time=20 ms)
In order to understand Eq. 5.6, several power levels ranging from 0.125 to 0.75 mW for the heat point source and with varying durations, ranging from 1 to 100 mS were evaluated. In this case, the distance \( (r) \) was varied until 100% healing was predicted. This approach was repeated manually for several time values.

Figure 5.6 shows the predicted weld size as a function of time for the various power levels. As expected, weld size is proportional to power level. It is interesting to note that after a particular length of heating duration \( (t_w) \), weld size is nearly independent of time. By evaluating the thermal histories for the various power levels, this observation can be explained by the fact that within a relatively short period of time, the system reaches near steady state. Thus, extending the duration of the heating does not significantly alter the temperature fields within the material.

It is seen that with a point heat source, welds as small as few hundreds of nm in radius are achievable.
Figure 5.6 Weld size as function of time for a point heat source (PS) at various power levels

It is interesting to note that this model predicts that nearly any minimum weld size can be produced with various power levels. That is to say, by reducing heating times, smaller welds can be produced.

In evaluating this model it is seen that the minimum weld size can be very small, less than 100 nm. In fact this size is so small that traditional squeeze flow models probably do not predict polymer flow. For example in traditional modeling of polymer flow, viscous flow is assumed. However the scale of 100 nm approaches the size of an
individual molecule. For example if a typical molecular weight of 700,000 g/mole is assumed for linear polyethylene, a de-natured chain pulled tight would be 11,000 nm long. Of course this configuration is thermodynamically impossible, and the chain would fold onto itself into much smaller configuration. In fact the molecule would fold onto itself in a dilute solution and form a crystalline lamellae that would be about 30 nm in thickness. Thus, again it is seen that molecular size and minimum weld size are of the same magnitude. Thus, in order to accurately predict minimum weld size, molecular mobility must be considered.

Another important aspect that must also be considered is surface effects. It was proposed by de Genness [61], that at a free surface, there is more free volume and more molecular mobility and thus diffusion can occur below Tg. This maybe important at a weld interface where asperity peaks keep some regions of the interface from making contact. Thus, with squeeze flow of the asperity peaks when these regions make contact, the molecules may already have a high level of free volume making healing easier than expected. In order to consider this effect, the surface roughness of several of the extrude sheets and films was measured. It was found that the peak to peak heights were between 0.15 μm and 0.25 μm and the distance between them was typically 50 and 100 μm. Thus, the faying surfaces had limited contact until squeeze flow of the asperity peaks occurred.

These limitations to the minimum achievable weld size are theoretical and assume that all other limiting factors, such as imperfections in the optics, non-parallel light sources and
material imperfections do not exist. These undesired limitations further increase the minimum weld size in the empirical experiments and represent the real world. In the following section, experiments are detailed that evaluate the minimum weld size based on real world limitations.

5.4 RESULTS OF DIFFRACTIVE OPTIC MICRO-WELDING

Using the experimental setup described in Figure 5.1, two lens systems for image reduction were evaluated:

1) 74 mm diameter double convex lens with focal length of ~64 mm (Oriel 12740)
2) 20x compound microscope objective lens

In the initial studies, a circular image with a 20 mm diameter was projected at the center of the 100 mm diameter lens (#1). It was found that better image resolution was obtained when the power was maximized and time minimized. This is expected, because these sets of parameters reduce thermal diffusion. However, it should be noted that these conditions may not minimize residual stresses within the weld. With this setup, the minimal weld circle diameter that was obtained was 1500 μm, see Figure 5.7. Because it is difficult to see the welds in the photograph, yellow circles are added to show their location. The circles correspond to the inner and outer diameters of the welds. In this case, the minimum weld width was approximately 200 μm. The circle diameter was
minimized by varying the work distance (distance between lens and weld). In this case, the working distance was 80 mm, slightly more than the focal length of the lens. Welds made at the focal length were simply spots and did not resemble the desired circular pattern. In this setup, the output of the laser was 80 W (47.2 W delivered at the weld) and the heating time was 5 ms. It is believed that smaller circular patterns were not achievable because of diffraction limited aberrations as detailed in Section 5.1.

![Figure 5.7 Microwelds with 100 mm diameter lens (PC substrate, 1 mm scale on top)](image)

In order to minimize limitations of image reduction, a 20 x compound lens system was used (lens #2). In this case, the microscope lens was illuminated with a circular image approximately 5 mm in diameter.
As seen in the burn pattern images in Figure 5.8, the resolution of the images was very good and in fact the resolution appears to approach the resolution of the ZAP paper (grain size of ZAP paper). In the first image (A), the working distance was approximately 7 mm and the circle diameter was approximately 600 $\mu$m. At the shorter working distance of 5 mm (B), the circle diameter was only 300 $\mu$m. Figure 5.9 shows a weld on PC made with 47.2 W of laser power from the DE and a weld time of 0.01 ms. It is seen that the fidelity of the weld is excellent and it appears to be as good as or better than the original images made without image reduction. This high resolution is probably due to increased image resolution with image reduction. In addition, it is seen that the weld diameter is approximately 300 $\mu$m and the weld width is about 75 $\mu$m. It is seen in the figure that there are finger link images extended outward from the center of the circle. Because of the location and geometry of these radial fingers, it is theorized they are the result of residual stress. These stresses are particularly noticeable in the center of the circle, where the PC film appears to have radial stresses originating from the center. The zero order
was masked from the image before it was focused as shown in Figure 5.1. It is believed that process optimization may help reduce these stresses. It is also seen that the aspect ratio of the weld line width and circle diameter is relatively large compared to convention welding (see Figure 2.42). That is to say, the weld width is large than expected. It is believed that this is due heat flow. Because the amount of heat per unit area required to make a weld is independent of weld size, with smaller welds there is relatively more heat diffusion which increases the relative line thickness.

Figure 5.9 Welds on PC with microscope lens 5 mm working distance
CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

In this study it was found that it was possible to use diffractive optics to reshape laser beams for TTIr welding of plastics. This is a novel and unreported method of making welds with plastics. In addition, it was demonstrated that images produced with diffractive optics could be resized with standard optics in order to make small welds (<300 μm). Again, another novel technique not reported. In addition, a novel rotating mask for photolithography was designed that allowed four level images to be etched on a substrate with a single mask. Other findings related to diffractive optics include:

- The process was relatively efficient (greater than 55%) and uniform welds could be produced.
- Diffractive lenses capable of transmitting more than 80 W of laser power were fabricated.
- In addition, weld times as short as 50 ms were achieved.
- With microwelding, weld times as short as 0.01 ms were achieved.
- Weld lines as narrow as 75 μm were achieved.
- 20 mm circle weld patterns could be generated that could sustain 0.7 MPa of air pressure without failure or leaking, which based on the weld geometry, results in...
an average weld stress of 16 MPa and near full parent strength near the edge of the weld

- Weld width was proportional to power and time.
- Excessive weld energy resulted in degradation at the weld center line.
- Weld geometries ranging from circle, squares and text were welded using diffractive imaging.

In terms of micro-fabrication, several key items were documented. For example, etch rates and quality of etching of fused silica with RIE. In addition, it was reported that etch depths with 10-30 nm resolution were achievable. One novel finding in terms of micro-fabrication was that it is possible to use one mask to etch multiple features in the same area (rotating mask).

It was also demonstrated that, while the weld process is very complicated and includes thermal transfer, molecular diffusion and squeeze flow, these models can be coupled into one model that accurately predicts the level (degree) of welding as well as weld size. It was also found that molecular healing models can be coupled with thermal models to predict minimum weld size.

Thus in summary, this work developed and characterized a new and novel technique for plastics welding using diffractive optics. It was proven that by using diffractive optics laser beams could be reshaped in order to create complex geometries for simultaneous welding of plastic in a through transmission infrared welding. This novel technique
included the use of standard optics for resizing diffractive image in order to make weld images in the range of a few microns. In addition, new molecular healing models were developed that accurately allowed the size and quality of a micro-welds to be predicted. This research opens new and novel technologies for the plastics and MEMS industry.

The final deliverables from this work, include but are but not limited to:

1. Demonstration of TTIr welding of plastics with diffractive optics
2. Demonstration that molecular diffusion activation energy is temperature-dependent
3. Developed coupled models for heat flow, squeeze flow and molecular diffusion for polymer interfacial healing
4. Two peer reviewed journal articles
5. Two patent applications

Below is a list of proposed areas that should be studied in the future:

1. Use optimized diffractive optics for TTIr welding
2. Optimize welding parameters for diffractive TTIr welding of plastics to maximize weld performance and reduce residual stresses. These parameter include but are not limited to:
a. Power
b. Time
c. Pressure
d. Laser beam distribution

3. Optimize holographic optics for TTIr welding plastics
   a. Further develop encoding technique
   b. Further develop illumination technique

4. Evaluated the use of micro-machined diffractive optics for laser welding of plastics

5. Develop models for healing based on the mobility of single molecules

6. Confirm that the aspect ratio of line width and image size increases with decreased weld size as a result of heat flow.
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APPENDIX A

MATH CAD FILE FOR DIFFRACTIVE DESIGN

Step 1: Read in image file

Step 2: Transpose the image from center to corners:

Divide the image into 4 equal parts

Invert the four equal parts
Put the 4 inverted parts back together
Top := augment(M00,M01)
Bottom := augment(M02,M03)

Step 3: Add random phase to target image
\[ \text{Phase}_{k,1} := -\pi + 2\pi \text{rnd}(1) \]
\[ \text{Mag}_{k,1} := |T_{\text{Target}}|_{k,1} \]
\[ \text{Real}_{k,1} := \text{Mag}_{k,1} \cos(\text{Phase}_{k,1}) \]
\[ \text{Img}_{k,1} := \text{Mag}_{k,1} \sin(\text{Phase}_{k,1}) \]
\[ C_{\text{Target}}_{k,1} := \text{Real}_{k,1} + i \text{Img}_{k,1} \]

Step 4: Take inverse complex FFT of complex target (C_{Target})
\[ F := \text{ICFFT}(C_{\text{Target}}) \]
This is the predicted mask, which has an infinite number of levels (256 displayed)

Step 5: Take the complex FFT of the magnitude of predicted mask:

\[
H := \left| \text{CFFT}(F) \right|
\]

\[
H := H
\]

We get a perfect circle!

But this is only possible if we use a very high level number of phases (number of etchings)

This is seen in the fact that the mask has many different grey scales, and for a two level mask it should be all black or white (2 level)

Step 6: We must truncate the phase of the predicted mask between pi/2 and 3pi/2 = 1 and 3pi/2 and pi/2 = 0

First we must calculate the phase of the mask (F):

The real part

The imaginary part

The phase angle

\[ \text{Mask Real}_{k,1} := \text{Re}(F_{k,1}) \]
\[ \text{Mask Imag}_{k,1} := \text{Im}(F_{k,1}) \]

\[ \text{Mask Phase} := (\text{arg}(F)) \]

Next we truncate the phase to 0 and pi (0 and 1)

\[
\text{Truncate}_{k,1} :=
\begin{cases}
0 & \text{if } 0 < \text{Mask Phase}_{k,1} \leq \frac{\pi}{2} \\
1 & \text{if } \frac{\pi}{2} < \text{Mask Phase}_{k,1} \leq \pi \\
0 & \text{if } -\frac{\pi}{2} < \text{Mask Phase}_{k,1} \leq 0 \\
1 & \text{if } -\pi < \text{Mask Phase}_{k,1} < -\frac{\pi}{2}
\end{cases}
\]

Step 7: Now we set the magnitude of the mask to one, and use the truncated phase
Also note that the magnitude is much less.

\[
\text{Mag}_{\text{CTarget}} := \sqrt{256^2} \\
\text{Mag}_{\text{CTarget}} = 256 \\
\text{Mag}_{\text{Mask}} := \sqrt{2^2 + \pi^2} \\
\text{Truncate}\_\text{Img} := \sin(\text{Mask}\_\text{Phase}) \\
\text{Truncate}\_\text{Real} := \cos(\text{Mask}\_\text{Phase}) \\
\text{Mask}\_\text{Truncate}_{k,1} := \text{Truncate}_{k,1} + i\cdot\text{Truncate}_{k,1} \\
\text{Mask}\_\text{Image} := 255\cdot\text{Mask}\_\text{Truncate}
\]

Mask\_Image

This is the mask in 2 levels

\[
\text{Mask}\_\text{ImageT} := 180\left(\left|\text{Mask}\_\text{Truncate}\right|\right) \\
\text{PImage} := \left(\left|\text{FFT}(\text{Mask}\_\text{Truncate})\right|\right) \\
\text{PImage} := \text{PImage}\_3900
\]

PImage

This is the predicted transposed target with a 2 level mask based on FFT of the mask x 2000

Step 8: Take the transpose of the predicted target image to see what we will really get:

\[
\text{PImage}_{0\_ll, kk} := \text{PImage}_{ll, kk} \\
\text{PImage}_{1\_ll, kk} := \text{PImage}_{ll, kk+24} \\
\text{PImage}_{2\_ll, kk} := \text{PImage}_{ll+24, kk} \\
\text{PImage}_{3\_ll, kk} := \text{PImage}_{ll+24, kk+24}
\]

Invert the four equal parts

\[
\text{M00} := \text{reverse}\left(\left(\text{reverse}\left(\text{PImage}_{0\_T}\right)\right)\_T\right) \\
\text{M01} := \text{reverse}\left(\left(\text{reverse}\left(\text{PImage}_{1\_T}\right)\right)\_T\right)
\]
M01

M00

M02 := reverse \left( \text{reverse}(\text{PImage}_2^T)^T \right)

M03 := reverse \left( \text{reverse}(\text{PImage}_3^T)^T \right)

M02

M03

Put the 4 inverted parts back together

Top := \text{augment}(M00, M01)

Bottom := \text{augment}(M02, M03)

Top

Bottom

PImage\_Final := \text{stack}(\text{Top}, \text{Bottom})

PImage\_Final
APPENDIX B

MATHCAD FILE FOR MOLECULAR HEALING

Read data files from impulse welds

°C = K

\( i := 0, 1 \ldots 50 \)

\( \Delta t := \frac{1}{50\text{Hz}} \)

\( t_i := i \Delta t \)

\( \theta_A := \text{C:\\}30A_16Sd.DAT} \)

\( \theta_B := \text{C:\\}30A_18Sd.DAT} \)

\( \theta_C := \text{C:\\}30A_19Sa.DAT} \)

\( \theta_D := \text{C:\\}point\_heat.DAT} \)

\( \theta_{PS} := \text{C:\\}point\_heat.DAT} \)
\[ \theta A := \theta A - 80^\circ \text{C} \]
\[ \theta B := \theta B - 80^\circ \text{C} \]
\[ \theta C := \theta C - 80^\circ \text{C} \]
\[ \theta D := \theta D - 80^\circ \text{C} \]

A goes from 39 to 49 (0%)
startA := 133
dendA := 144

B goes from 156 to 193 (43%)
startB := 136
dendB := 157

C goes from 174 to 207 (61%)
D goes from 160 to 177 (OW%)

startC := 134
dendC := 166
startD := 138
dendD := 171
startPS := 33
dendPS := 47

\[ K1 := 205 \times 10^{-11} \text{J} \]
\[ K2 := 1040 \text{^\circ C} \]
\[ \text{Dau}_0 := 0 \]

\[ EA(\theta A) := K1 \cdot e^{(\theta A)} \]
\[ EB(\theta B) := K1 \cdot e^{(\theta B)} \]
\[ EC(\theta C) := \frac{K_2}{1 + e^{-(\theta C)}} \]
\[ ED(\theta D) := \frac{K_2}{1 + e^{-(\theta D)}} \]
\[ A_i := \text{start}_A, \text{start}_A + 1, \ldots, \text{end}_A \]
\[ K_0 := 7.5 \times 10^{-4} \text{ sec}^{-1} \]
\[ K_{A_i} := \frac{1}{K_0} e^{-K_0 \theta A_i} \]
\[ we \ need \ 0-1 \]
\[ \text{Dau}_A := \text{Dau}_0 + \sum_{j=\text{start}_A}^{\text{end}_A} K_{A_j} \Delta t \]
\[ \text{Dau}_A \cdot 100 = 0 \%
\]
\[ \text{B}_i := \text{start}_B, \text{start}_B + 1, \ldots, \text{end}_B \]
\[ K_{B_i} := \frac{1}{K_0} e^{-K_0 \theta B_i} \]
\[ \text{Dau}_B := \text{Dau}_0 + \sum_{j=\text{start}_B}^{\text{end}_B} K_{B_j} \Delta t \]
\[ \text{Dau}_B \cdot 100 = 18.863 \%
\]
\[ \text{C}_i := \text{start}_C, \text{start}_C + 1, \ldots, \text{end}_C \]
\[ K_{C_i} := \frac{1}{K_0} e^{-K_0 \theta C_i} \]
\[ \text{Dau}_C := \text{Dau}_0 + \sum_{j=\text{start}_C}^{\text{end}_C} K_{C_j} \Delta t \]
\[ \text{Dau}_C \cdot 100 = 36.778 \%
\]
\[ \text{D}_i := \text{start}_D, \text{start}_D + 1, \ldots, \text{end}_D \]
\[ K_{D_i} := \frac{1}{K_0} e^{-K_0 \theta D_i} \]
\[ \text{DauD} := \text{Dau}_0 + \sum_{j = \text{startD}}^{\text{endD}} \frac{1}{4} \cdot \text{KD}_j \cdot \Delta t \]

\[ \text{DauD} \times 100 = 60.384 \]

80%