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FINAL REPORT

ON

BONDING LARGE AREA SILICON WAFERS

CONTRACT NO. 952022

PREPARED FOR

JET PROPULSION LABORATORY

4800 Oak Grove Drive

Pasadena, California 91103

PREPARED BY

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ABSTRACT

The materials and processes necessary to make reliable, large area bonds have been investigated. Emphasis has been placed on three aspects of bonding wafers larger than 1 inch:

(a) Bonding Processes - Five techniques for bonding wafers have received attention.

- (1) Diffusion Bonding - High temperature metallic bonds with low temperature methods have been the principal study. Reasonable success has been achieved in applying this process to 1-inch and 2-inch wafers bonded to molybdenum heat sinks.
- (2) Amalgam Bonding - An adaptation of diffusion bonding was also studied.
- (3) Eutectic Soldering - A method by which small area die bonds are made was attempted in the large area case.
- (4) Filled Epoxy Bonding - Organic binders filled with metallic elements were used to form strong and reasonably conductive large area bonds.
- (5) Anodic Bonding - The use of heat and electric field produced exceptionally strong bonds between metals and glasses.

(b) Properties of Liquid-Solid Bonding Materials - Indium, tin, and lead combined with silver or gold form binary compounds often encountered in metallic bonding. Coefficient of expansion, thermal conductivity, elastic modulus and tensile strength have been measured for the binary system Ag-In, which typifies alloys formed in diffusion bonding. Expansivity and conductivity are also reported for five commonly used eutectic systems.

(c) Stress in Joined Bodies - A calculation has been done which approximates the stresses present when a bond between materials of unequal expansivity is made. The approach employs the principle of superposition using applied tensile forces in place of the surface shear present in the bonded system. Results are presented for the radial, azimuthal and axial components of stress in a tri-layer wafer-to-heat sink bond.

The study has shown that mechanically strong bonds can be made between silicon wafers whose diameter exceeds 1-inch and molybdenum heat sinks. Using a Pb-Sn-In solder and the diffusion bonding method it is possible to achieve bonds whose decomposition temperature is in excess of 400°C in spite of the fact that the bonding temperature is only 250°C. The advantage of this method over existing soldering schemes lies in the fact that stresses due to thermal excursion are kept low while a high temperature bond is still achieved.

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SECTION I

1.0 INTRODUCTION

This report describes work performed during an 18-month program to develop techniques for reliable bonding of large area wafers to suitable heat sinks. The purpose is to enable bonding silicon single crystals of up to two inches in diameter in a manner which does not damage the wafer, or affect the performance of devices contained therein. The provision of a path of low thermal resistance between the heat sources and the heat sink is an essential character. The materials of the system should not degrade under continuous operation, or show deleterious effects when subjected to thermal shock or other high stress testing.

The problem has been approached in three phases. The first is the study of potential large area bonding processes. Herein five distinct types of large area bonding methods are discussed.

Diffusion Bonding - This is a method of producing high temperature bonds with low temperature processing. Investigations into solid state and liquid state methods are reported. The solid state bonds make use of the principle of the diffusion couple with solid state diffusion as the mechanism. The liquid state bonds rely on a liquid-to-solid transition occurring as a high melting point material dissolves in a lower melting point one.

Amalgam Bonding - This method is similar to diffusion bonding except a high temperature metal is dispersed throughout a liquid metal layer. Annealing produces dissolution of the high melting point material, and hardening results. This is the principle underlying the common dental filling and has shown promise in this bonding application also.

Eutectic Soldering - Used today to make many die bonds, this method involves heating materials which form a binary eutectic while holding them in intimate contact. The liquid layer formed is the solder which holds the bonded components together when it solidifies.

Filled Epoxy Soldering - By dispersing metallic elements within an epoxy binder, the adhesive properties of the epoxy can be retained while enhancing its thermal conductivity. Since this is a requirement of a large area bond, such a system was investigated.

Anodic Bonding - Temperature and the electric field can be employed to make a high quality bond between metal and glass, well below the softening point of the glass. The ability to match the expansion coefficient of glasses to the particular metals used, makes the system attractive.

Measurements of pertinent thermophysical properties of bonding materials comprised the second phase of the program. A knowledge of parameters such as expansion coefficient, thermal conductivity, tensile strength, and elastic modulus can save time and effort in matching the binder to the job, in addition to providing a more reliable system. These data have been obtained for the Ag-In system which typifies the systems used in diffusion bonds, and also for several eutectic solder alloys.

The third phase has been devoted toward the evaluation of stress levels on bonded systems. After an initial attempt at numerically approximating the problem, an analytical approach to the problem was applied. By employing the principle of superposition and an "all-tensile-force" model, reasonable solutions for the required stresses were obtained. Although not strictly correct, in that certain forces are neglected, the general approach appears to yield a practical solution to an otherwise very complex mechanical problem.

SECTION II

2.0 ANALYSIS OF WORK

Emphasis during this project has been placed in three areas. The first is the investigation of techniques for making a high quality bond between two large area wafers, or between a wafer and an appropriate heat sink. The second is the determination of various thermophysical properties of some currently used bonding materials, and also of a system which typifies prospective future "solders." The third is to analyze in a "quasi-theoretical" manner, the stresses which occur when such large area bonds are made.

2.1 DIFFUSION BONDING

To bond large area silicon to heat sinks, it is becoming apparent that nonstandard bonding techniques must be employed. This is because:

- (1) Low temperature bonding must be invoked to minimize stress due to the disparity of thermal expansion coefficients between silicon and heat sink materials.
- (2) Hard solders with elevated melting points must be employed. They must possess high elastic limits to prevent embrittlement due to work hardening of the solder.

An attractive solution of this apparent dichotomy is to employ diffusion bonding techniques wherein the bond can be made at relatively low temperatures, but the resultant bonding material will possess desirable mechanical properties, and will melt only at temperatures in excess of the bonding temperature. The diffusion

process is a particularly attractive bonding method for joining silicon to a heat sink, since thin films of metals can be employed as the bonding material requiring relatively short times for the diffusion process to become complete.

Two basic classes of diffusion bonds have been investigated throughout this project. These are discussed in detail in the following subsections.

2.1.1 Liquid State Diffusion Bonds

Several binary metallic systems exist in which one component has a low melting point and the other a high one. Typical of these are the Au-In⁽¹⁾, Au-Sn and Ag-In systems. Phase diagrams for these are shown in Figures 1, 2, and 3. Ternary and quaternary combinations of Pb, Sn, In and Au or Ag also display similar behavior.

By examining the phase diagram, one can see how these systems can be used at low temperatures to establish a bond which is stable to much higher temperatures. Consider as an example, the Au-In diagram shown in Figure 1. Suppose a thin layer of indium is placed in contact with a thicker layer of gold and the system annealed at some nominal temperature, say 250°C. Initially, the indium will become liquid and dissolve a given quantity of gold, determined by the composition at which the 250°C isotherm crosses the liquidus curve, (in this case about 2 atomic percent). The diagram also shows that this liquid is separated from the solid gold by several layers namely the γ , γ' and ζ solid phases and the solid compounds AuIn, and AuIn₂. As time-at-temperature progresses, the diffusion of gold through these layers will cause the complete transformation of the liquid into a final layer of AuIn₂, at which time the melting point of the system is greater than 450°C,

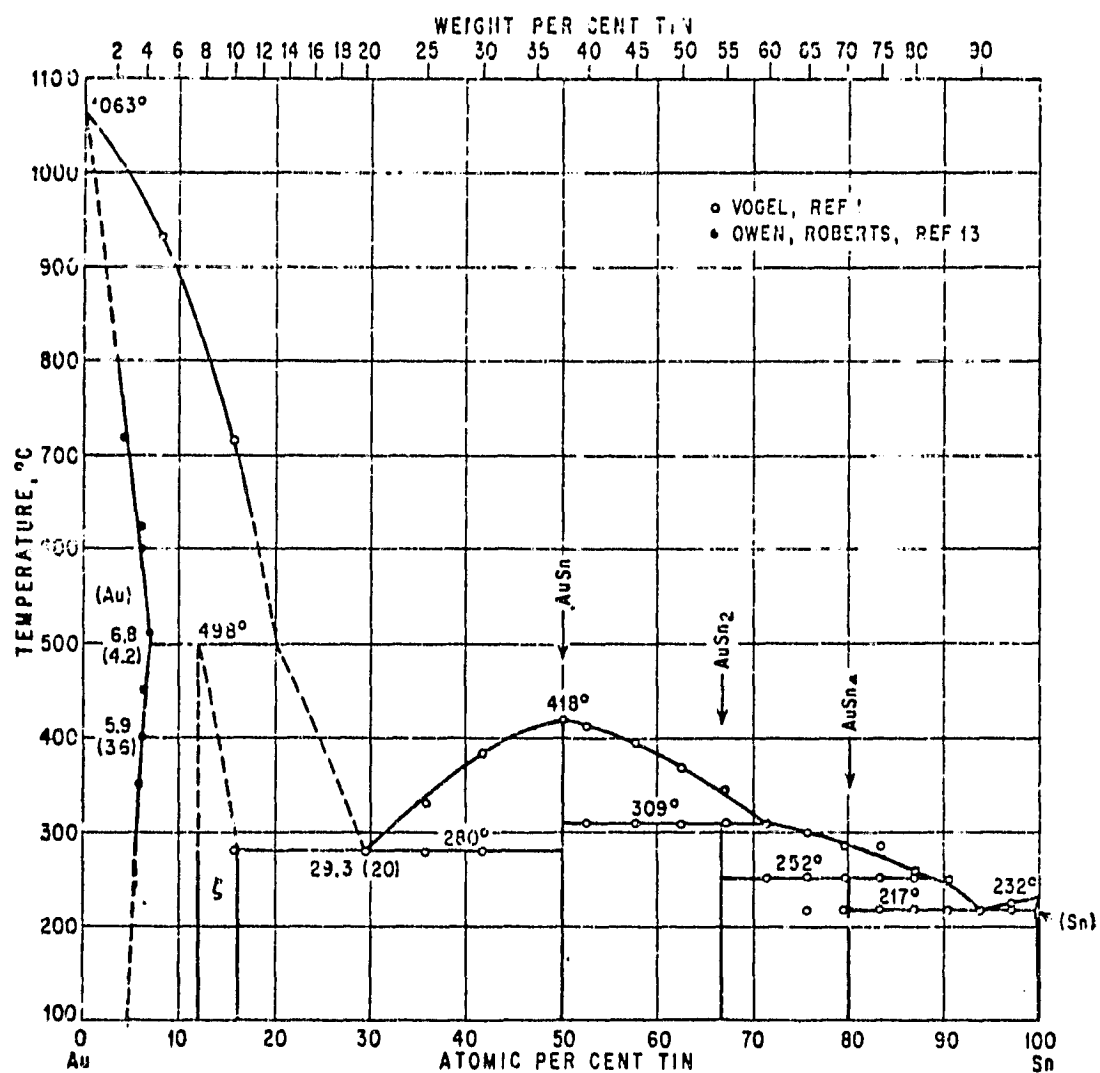


Figure 2. Phase Diagram for Gold-Tin

the eutectic decomposition point of the 40 percent In solid. If the anneal is continued, solid state diffusion drives the mixing until equilibrium and a single phase is reached. This is determined by the initial amounts of either material which exists. Ideally, initial layers should have a Au/In ratio of about 9 to insure a final solid in the gold solid solution region and a melting point greater than 700°C. In practice, however, the time for reaching a single phase is much greater than practicality allows and the useful bond contains several intermetallic layers.

In the Ag-In system, a similar analysis shows the bond temperature; just after solidification occurs, to be in excess of 600°C, the decomposition point of the ζ phase. If the Au-Sn system anneal is carried out above 300°C, the decomposition point should be about 500°C. For ternary and quaternary systems, exact decomposition points can only be determined by experiment.

The bonding process itself, then, proceeds in three distinct phases. First, the liquid metal must wet and dissolve some of the higher melting point material. If the materials are incompatible such that the liquid does not wet the solid, or there is no mutual solubility (even if only in limited quantities), then the bonding cannot proceed. Secondly, interdiffusion between the liquid and solid results in the gradual solidification of the liquid to a higher melting point compound. Lastly, solid state diffusion is the only mechanism driving the bond to equilibrium after solidification has occurred.

2.1.2 Bonding Procedures

The substrate materials chosen for this project were molybdenum and tungsten because their thermal expansion coefficients closely match that of silicon. Table I shows possible candidates

TABLE I

Material	Exp. Coeff. (ppm/ ^o C)	Therm. Conductivity (CGS units)
Si	3.2	0.2
Kovar	5.7-6.2	0.04
Cu	18.2	1.0
Au	14.3	0.7
Ag	18.8	1.0
Al	23.3	0.5
Mo	5.5	0.3
W	4.6	0.47

for heat sinking materials with their thermal conductivities and expansion coefficients. To optimize both parameters simultaneously the choice of tungsten should be made, but difficulties in electroplating tungsten with gold and silver led to the choice of molybdenum. The molybdenum substrates were polished flat and electroplated from a citrate-acid bath with a 0.5 mil layer of Au. This plating is followed by a 1000°C anneal in dry H₂ to enhance the adherence of the gold plate to the molybdenum.

The wafers were prepared by the following process:

- (1) Backside buffered etch with HF to remove any silicon dioxide film just prior to step 2.
- (2) Vacuum deposit 0.3 micron of gold on the back of the silicon wafer.
- (3) Alloy the gold to the silicon by raising the gold-silicon couple to 400°C in N₂ or forming gas to form a near eutectic alloy composition. This provides intimate contact between the gold and silicon resulting in good adherence. The wafer is then quenched from the alloying temperature to room temperature to form highly dispersed and tiny silicon crystallites distributed throughout the gold. The quench enhances adherence of an electroplated gold to the eutectic alloy.
- (4) HF etch the backside again to reduce native oxide thickness and silicon crystallites. This also enhances adherence between plated and alloyed gold.
- (5) Electroplate gold onto the gold-silicon eutectic to a thickness of 0.5 mil.

The low melting point material (i.e., indium, tin, lead or some combination) is then applied either as an electroplated layer or in the form of a solder preform. Initially, only electroplated layers were used but the presence of voids attributed to contaminants from the plating process led to the use of metallic preforms which were rolled to about 1 mil. This will be discussed further in 2.1.3, Part b. The use of preformed discs also allowed experiments with a wider variety of low melting point alloys than could be achieved by electroplating. In many cases it is simply a matter of rolling commercial solders, which have predetermined wetting characteristics, and cutting the required shapes.

The silicon is then clamped under pressure to the preform (or plated layer) and the gold-plated substrate, and placed into a furnace where it is heated at the desired temperature under a forming gas ambient.

It is especially important that the clamp not be removed and that the specimen is not cooled before the entire liquid phase disappears. If it is removed prematurely from the oven, the wafer will buckle and large voids will occur.

2.1.3 Problems Associated with Large Area Bonds

Since the area over which a uniform bond must be achieved is great for large wafers, the problems of making the bonds are amplified. In smaller area die bonds where eutectic soldering is employed, "scrubbing" the wafer to break up oxide layers and to eliminate voids is possible. This is not feasible with the large area bonds and voids are a major problem. The larger wafers are also easily marked during preparation and these defects may result in cracks upon cooling after a bond is made.

(a) Wafer Cracking

Initial experiments with 2-inch diameter, 7 mil thick wafers were very unsuccessful because during the cooling process, the wafers were severely cracked. Many experiments were done wherein the wafer was watched as it cooled from 250°C to room temperature. In several cases it was observed that when the wafer cracked it was from an edge, and closer inspection revealed a chip or scratch at the point where the crack began. In other cases, no defects were observed but cracks persisted.

The problem was eventually overcome by two methods. It was found that the use of thicker wafers (15 to 20 mils) eliminated the cracks. When this was not possible, the use of wafers of exceptional quality with low dislocation densities and no apparent surface defects also eliminated the cracking. Many 1-1/4 to 2 inch wafers have been bonded by the methods described herein and the cracking problem has been eliminated.

(b) Voids in Solid-Liquid Diffusion Bonds

The major problem encountered in this program has been the presence of large voids in the solder layer. Examples of some voids are shown in the photomicrographs of Figures 4, 5 and 6. These voids, in liquid-solid bonds are generally of two types; smooth-walled spherical voids randomly distributed, near the center of the wafer (Figure 4); and elongated irregular voids running parallel to the interface (Figure 5). In extreme cases, voids encompassing up to 50 percent of the solder volume have been seen (Figure 6).

It is possible to enumerate a variety of causes for void formation in solid-liquid bonding:



Figure 4. Smooth-Walled Voids in a Liquid-Solid Bond

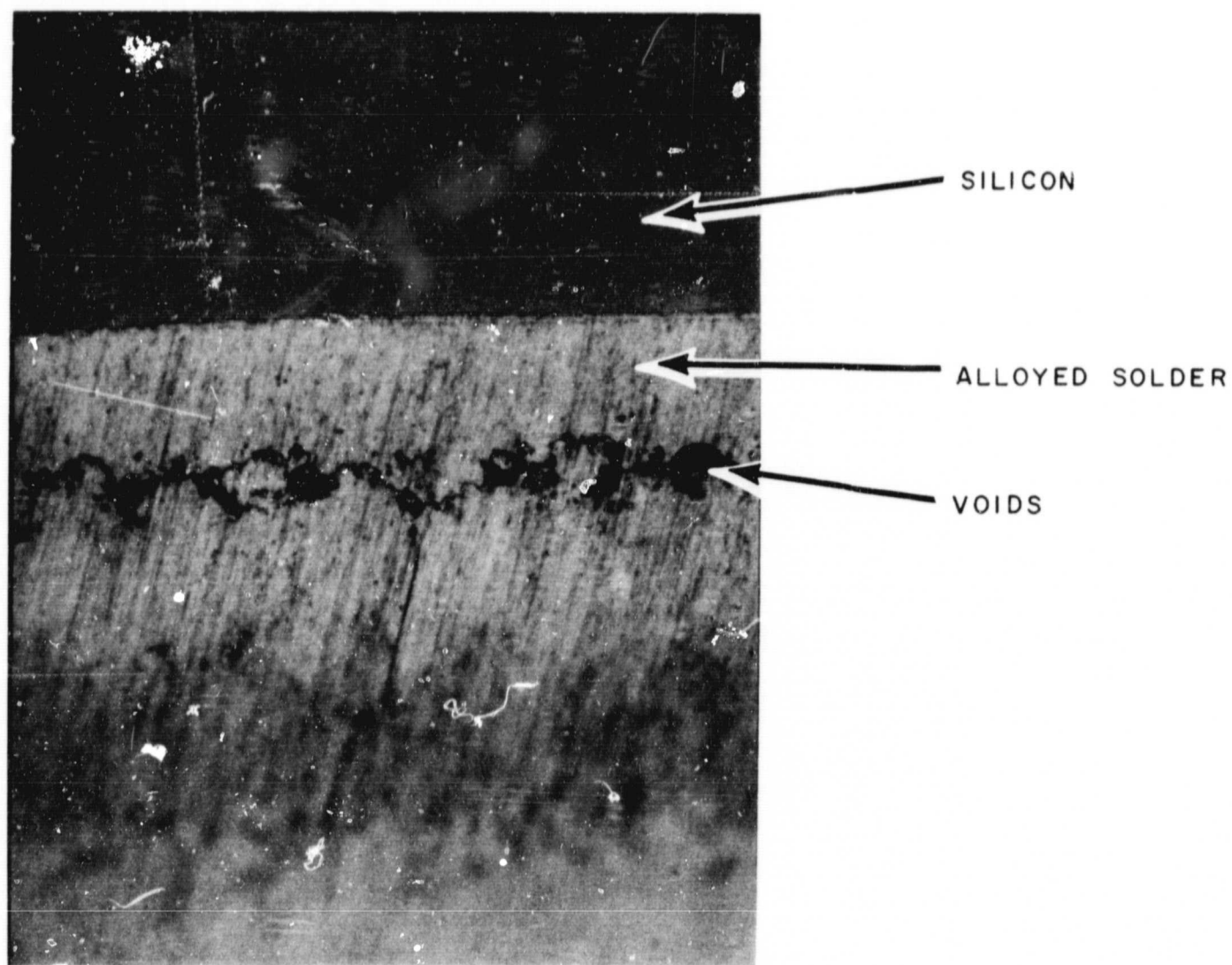


Figure 5. Voids in a Au-In-Au Bond

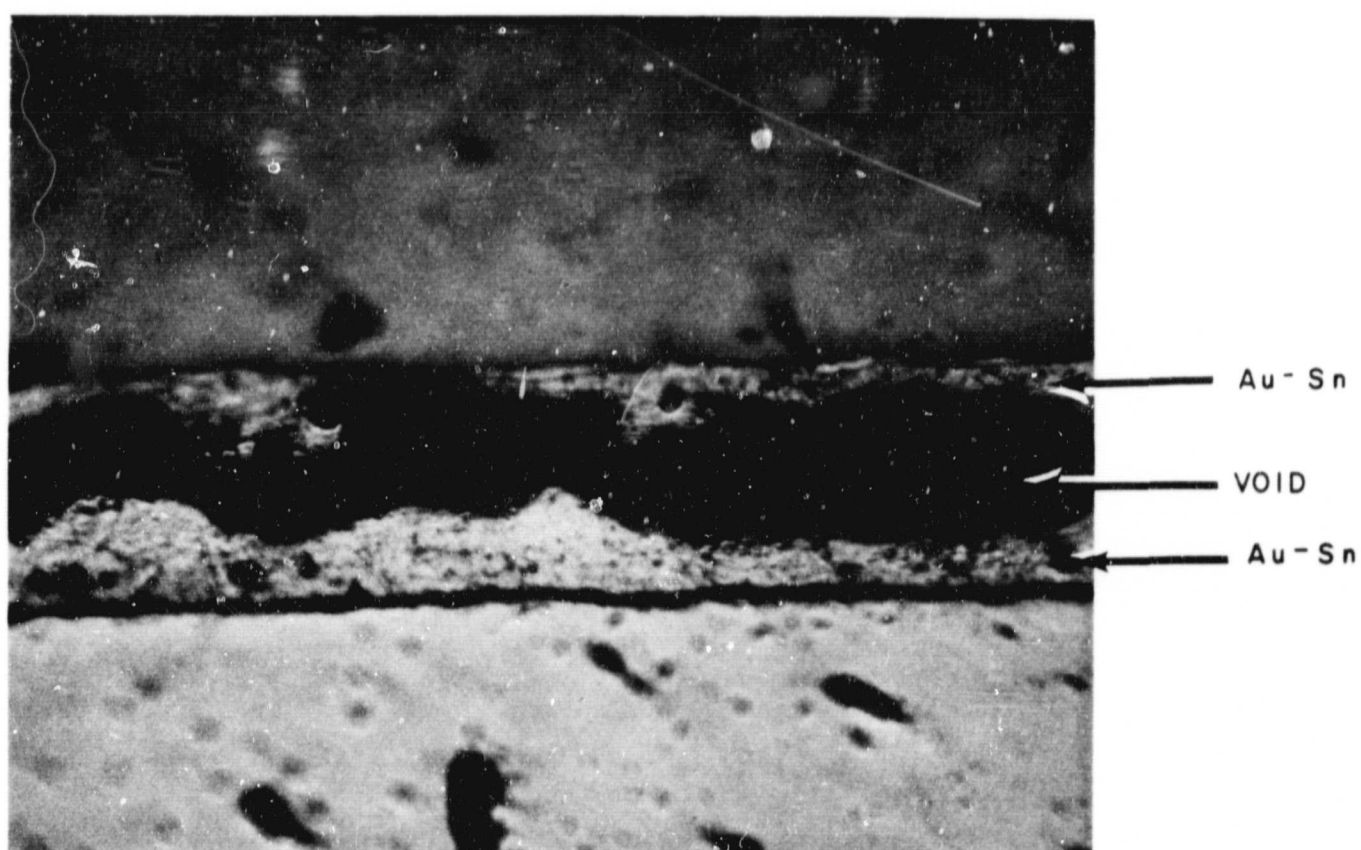


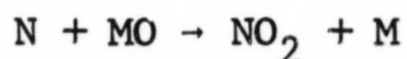
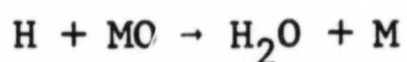
Figure 6. Large Voids in a Liquid-Solid Bond

(1) Trapped Gas- Since the electroplated layers of material are rough textured, small pockets of air are trapped between the wafer and substrate when they are placed in contact before the diffusion anneal. When the low melting point layer wets, this trapped gas becomes a bubble in the solder. These may appear as smooth-walled spherical holes along the initial bond interface and should be more prevalent near the center of the wafer, where the chance of gas escape is very small.

(2) Outgassing- Because of the initial method used for making the metal layers, namely electrodeposition, from a cyanide bath containing organic brighteners, a significant amount of gas, and even possibly liquid, may be included in the films. When the center layer wets out, these gases evolve (the liquids vaporize) and form voids similar to those of the trapped vapor but located within the liquid material rather than along the initial interface.

(3) Nonuniform Cooling- It has been observed that the cooling process proceeds from the outer edges of the bonded wafer to the center. If the wet layer has not completely solidified upon removal from the annealing furnace, then the faster cooling at the edge "pins" it to the substrate. Further cooling causes the central region to bulge, due to the disparity in expansion coefficient, and "pillaring" of the unsolidified material in this region may occur. Alternate regions between connecting pillars appear as voids (Figure 7).

(4) Chemical Reaction- The presence of metallic oxides in the deposited layers may cause the release of gases when N_2 and H_2 are present. Through the reactions



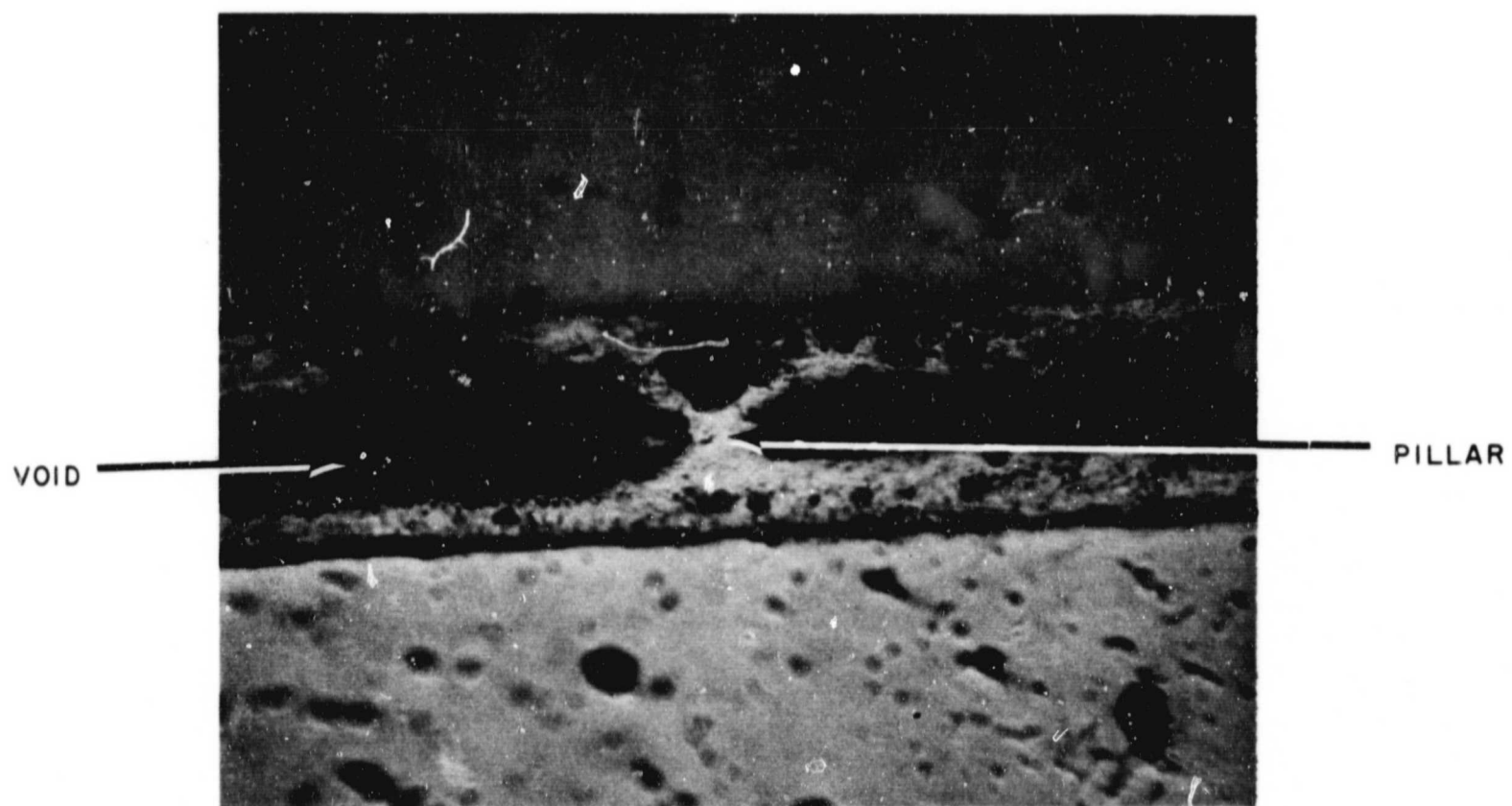


Figure 7. Pillaring in a Liquid-Solid Bond

steam and nitrous oxide may evolve and form the gas filled voids previously described.

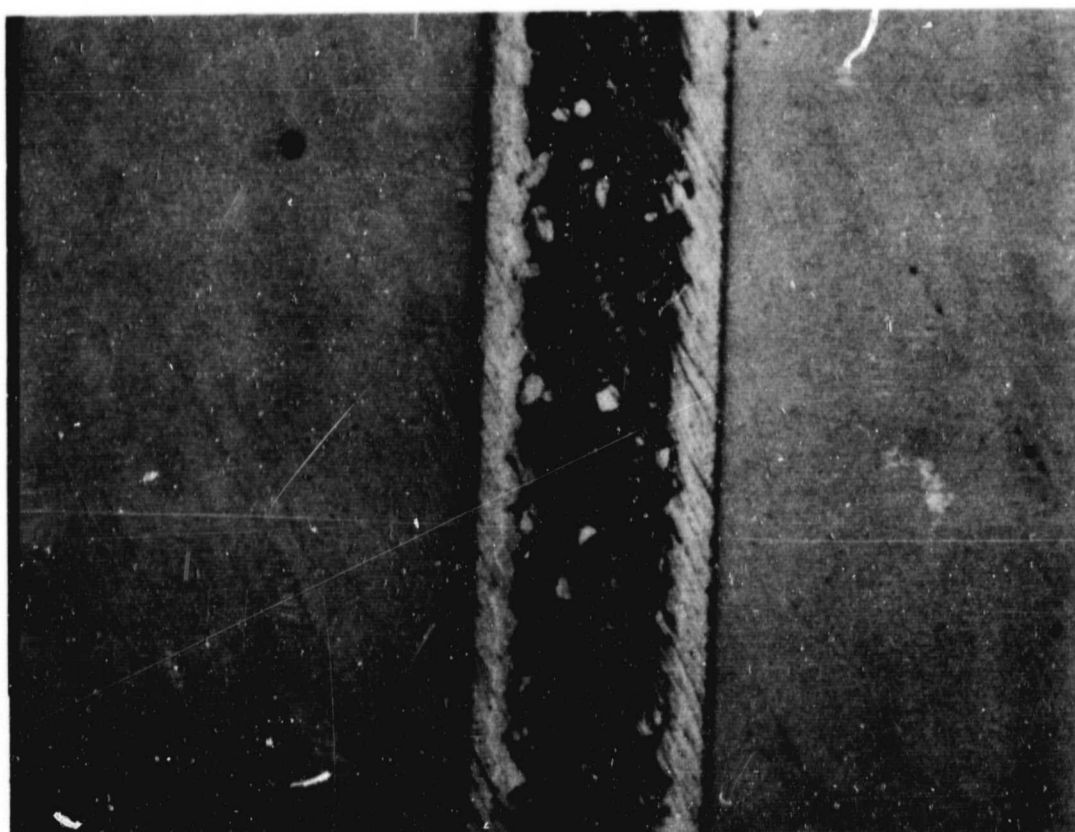
(5) Dewetting- In systems where non-mating surfaces are put together (e.g., indium on the wafer and tin on the substrate), one surface may dewet leaving long wide voids along the initial interface.

(6) Diffusion Effects- If the diffusion anneal is continued after hardening, small voids may evolve due to the anisotropy in diffusion coefficient across an interface (Kirkendall effect⁽²⁾). Other small voids may result from the clustering of vacancies and dislocations which are probably present in large numbers in electroplated films. Both of these effects are probably quite insignificant when compared with the others.

2.1.4 Results

As a first attempt at finalizing a process without the deleterious void problem, the use of the electroplated layer was eliminated. This removed any trapped organics and gases from the center layer. As a replacement thin preforms of pure indium and pure tin were used. These were rolled flat, varied in thickness from 1 to 4 mils, and were sandwiched between the wafer and heat sink. The use of 99.999+ percent pure metals also guaranteed freedom from impurity oxides along with eliminating the troublesome organics. Anneal temperatures were 250°C for the In system and 300°C for the Sn system for less than one hour.

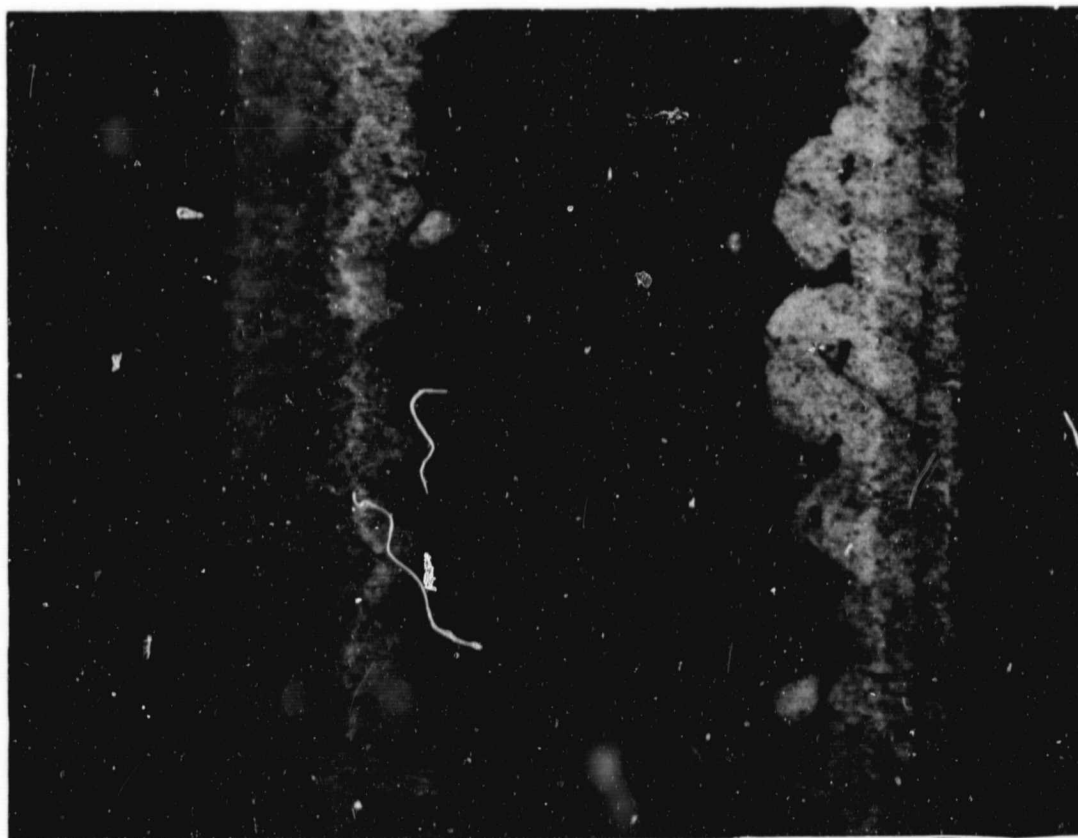
Figures 8 and 9 show a cross section through a 1.5-inch wafer-wafer bond using Au-In-Au. The entire bond segment is shown to be void free and the formation of high melting point intermetallics is evident. It is clear, however, that alloying is incomplete;



250X

Figure 8. Cross Section Through a Au-In-Au
Solid-Liquid Diffusion Bond

7620-10-8



1000X

Figure 9. Cross Section Through Au-In-Au
Solid-Liquid Diffusion Bond
Showing Alloying and Intermetallic
Formation

7621-10-8

the center of the bond is probably pure indium, and the need for still thinner preforms (the original preform was about 4 mils) is evident. Measurements show that complete alloying occurs to just over 1 mil at the time-temperature used and this seems to be the upper limit on the preform thickness.

In spite of this, however, the absence of the previously seen gas-pocket voids is gratifying. The use of the "impurity-free" preforms has provided a solution to problems 1 and 2.

Pillaring (problem 3) has been eliminated by allowing complete hardening of the bond layer before unclamping. It was suspected that when a bond is unclamped and cooled while the solder in the center is still liquid, buckling of the wafer may occur due to unequal expansion between the heat sink and wafer. It is this buckling which causes pillaring. Allowing the bond to completely solidify has eliminated this problem, and it is an essential step in producing a good high temperature bond.

It is a well-known fact that the addition of impurities to a normally pure liquid metal decreases the surface-free energy of the melt, making the wet and flow process proceed in an easier fashion. In addition, diffusion in an alloy may proceed faster than in either of the parent materials (although this is not always true). With this idea in mind, alloy solder preforms for the wet layer which we have been developing, manifests superior "wet and flow" characteristics. In most applications where preforms are used, flow of the solder is not desirable although good wetting of the surface to be bonded is essential. At present, bonds employing pure electroplated Au from an acid-citrate bath and the ternary system Pb-In-Sn (37.5%, 25%, 37.5%) have been found to work best. This commercially available solder melts at 138°C, wets exceptionally well on Au, and alloys quickly to a high temperature bond (Figure 10). Bonding tests

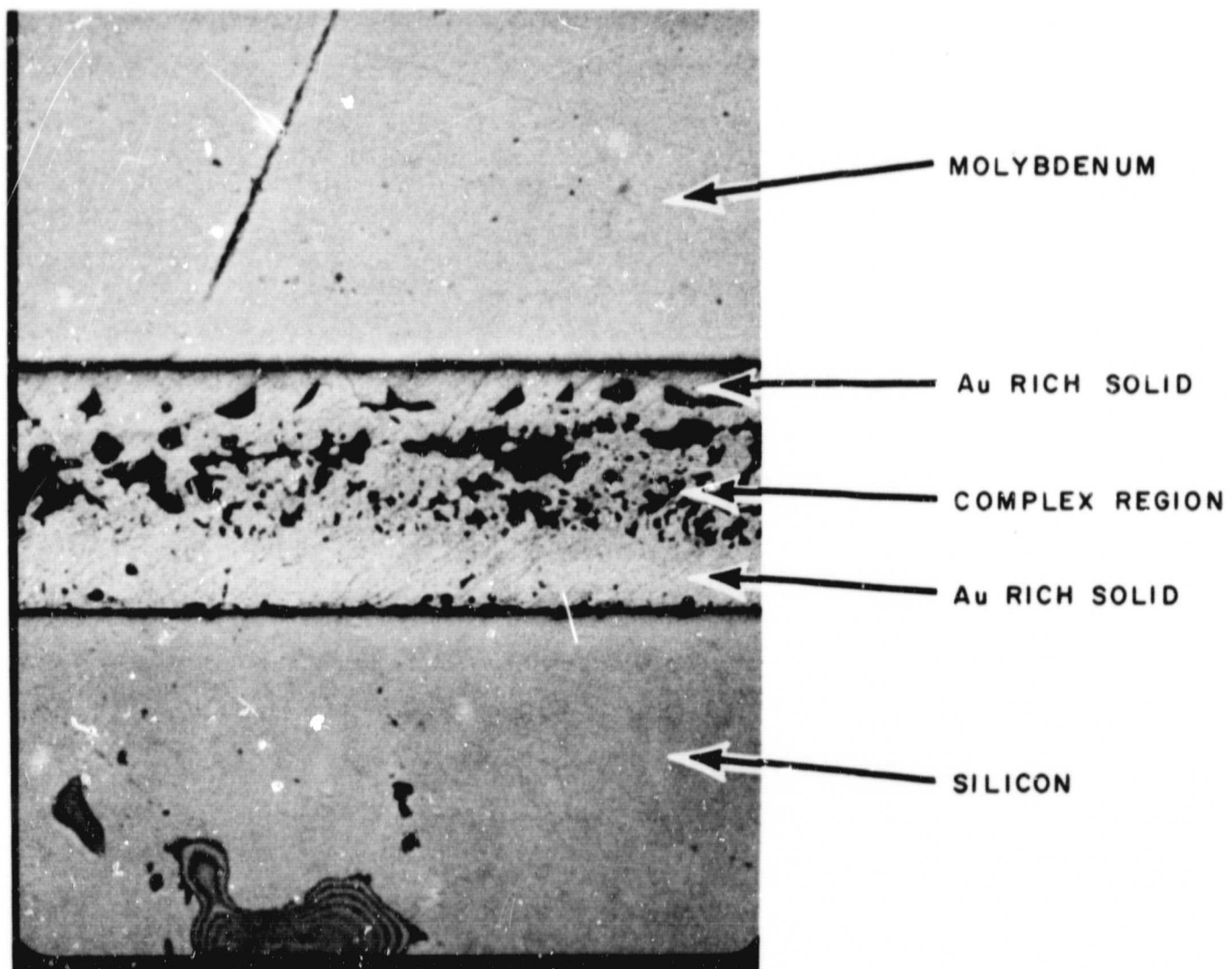


Figure 10. Diffusion Bond Using Pb-Sn-In
One-hour 250°C

7794-1-9

have been performed at temperatures to 400°C and no re-melt or decomposition is apparent after alloying is complete. Shear tests performed on several samples show the weakest part of the system to be molybdenum-gold interface. In every case where alloying is complete, shearing at levels of about 3000 psi caused the entire bonded region to be stripped clean from the molybdenum substrate.

A complete tabulation of the important systems used in liquid state bonding with Au is given in Table II with appropriate comments as to their performance.

TABLE II

System (Melting Pt.)	Decomposition Point	Composition (%)	Comments (Bonds made at 300°C, 1 hr)
Au-In-Au (155°C)	451°C	100	Plated: low shear strength many voids complete alloying Preform: no voids less than 1 mil for alloying
Au-Sn-Au (232°C)	418°C	100	Plated: solder is hard but has many large voids Preform: wets-fair; intermetallics crack Si
Au-(Pb-Sn-In)- Au (138°C)	>400°C	37.5, 37.5, 25	Preform: wets-excellent voids small & few strength: greater than plating on Mo
Au-(Pb-Sn-In- Cd)-Au (125)	>400°C	10, 15, 70, 5	Preform: about same as Pb-Sn-In

2.1.5 Testing Liquid State Bonds

Mechanical tests of the bonds were performed by soldering flat molybdenum discs together in an overlapped fashion and pulling in the Instron tester described below. In almost every case, the bond strength surpassed the strength of adherence of the gold film to the molybdenum plate.

Electrical performance testing was done on a few bonded specimens. Wafers one inch in diameter containing power transistors were bonded to heat sinks. No degradation or decrease in beta was observed. SCR devices bonded with this method showed only slight degradation.

Non-destructive tests need to be performed for production line testing for bond quality. One such testing procedure was developed during this contract. It involves the use of liquid crystals for determining hot spots which result from voids and unreliable wafer bonds. Figure 11 shows a schematic drawing of the experimental set up. The bonded wafer is heat sunk beneath the substrate, (this is either an ice bath or thermoelectrically controlled panel), and simultaneously heated from above. Liquid crystals, mixed to respond in the appropriate temperature range are applied to the top of the wafer. Since the voids constitute a higher resistance path to the heat sink than the well-bonded regions, hot spots will occur above them. These spots will then appear at a different color than the rest of the wafer. Examples of a two inch wafer which has one side well bonded, while the central region is very badly voided are shown in Figures 12 and 13. At present the resolution of voids is only fair, (voids must be about 4 to 5 times larger in diameter than the distance between the voids and the liquid crystal before they are detectable); but further experience with new liquid crystals is expected to improve this, and the use of this method as a valuable testing tool will be applied in the future.

Thermal cycling tests have been performed on several one inch wafers bonded to 1-1/4 inch molybdenum heat sinks. The range of temperature used was -70°C to +170°C. Tests were conducted

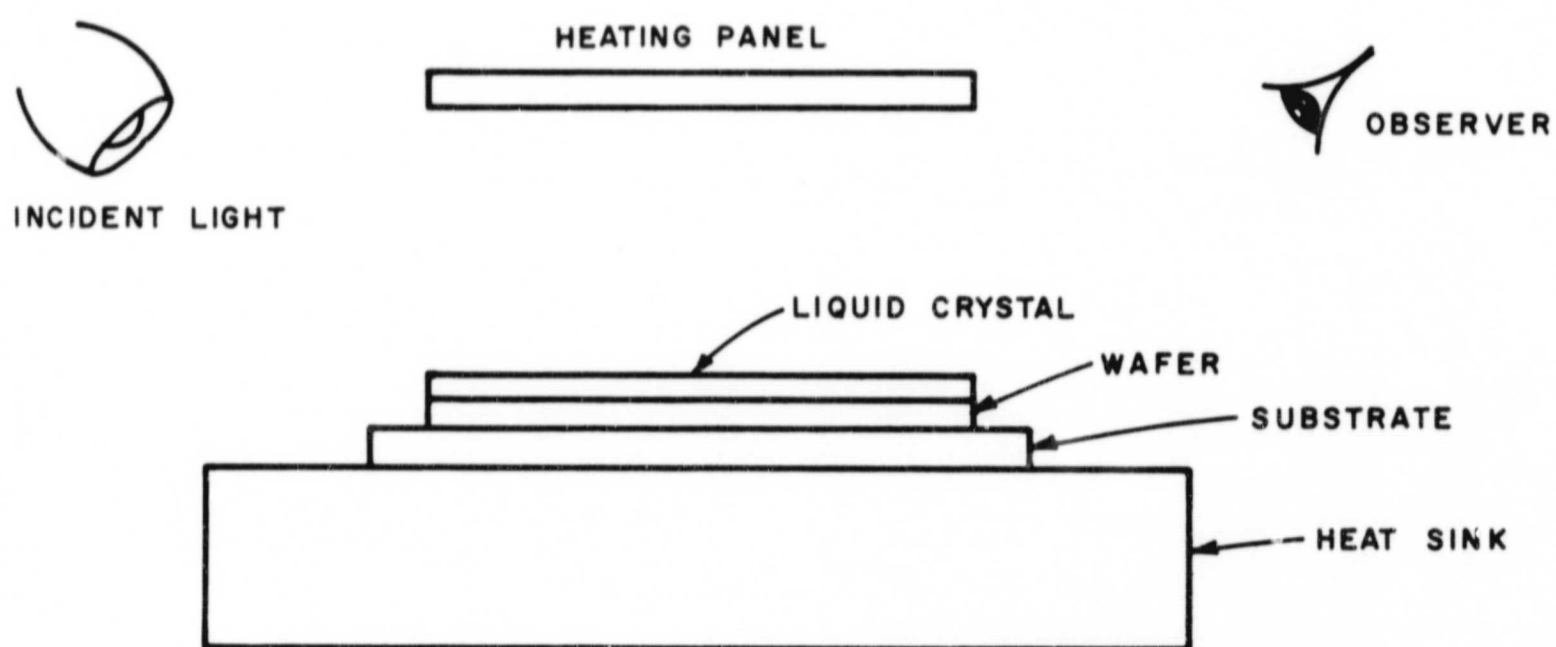


Figure 11. Schematic of Liquid Crystal Test System

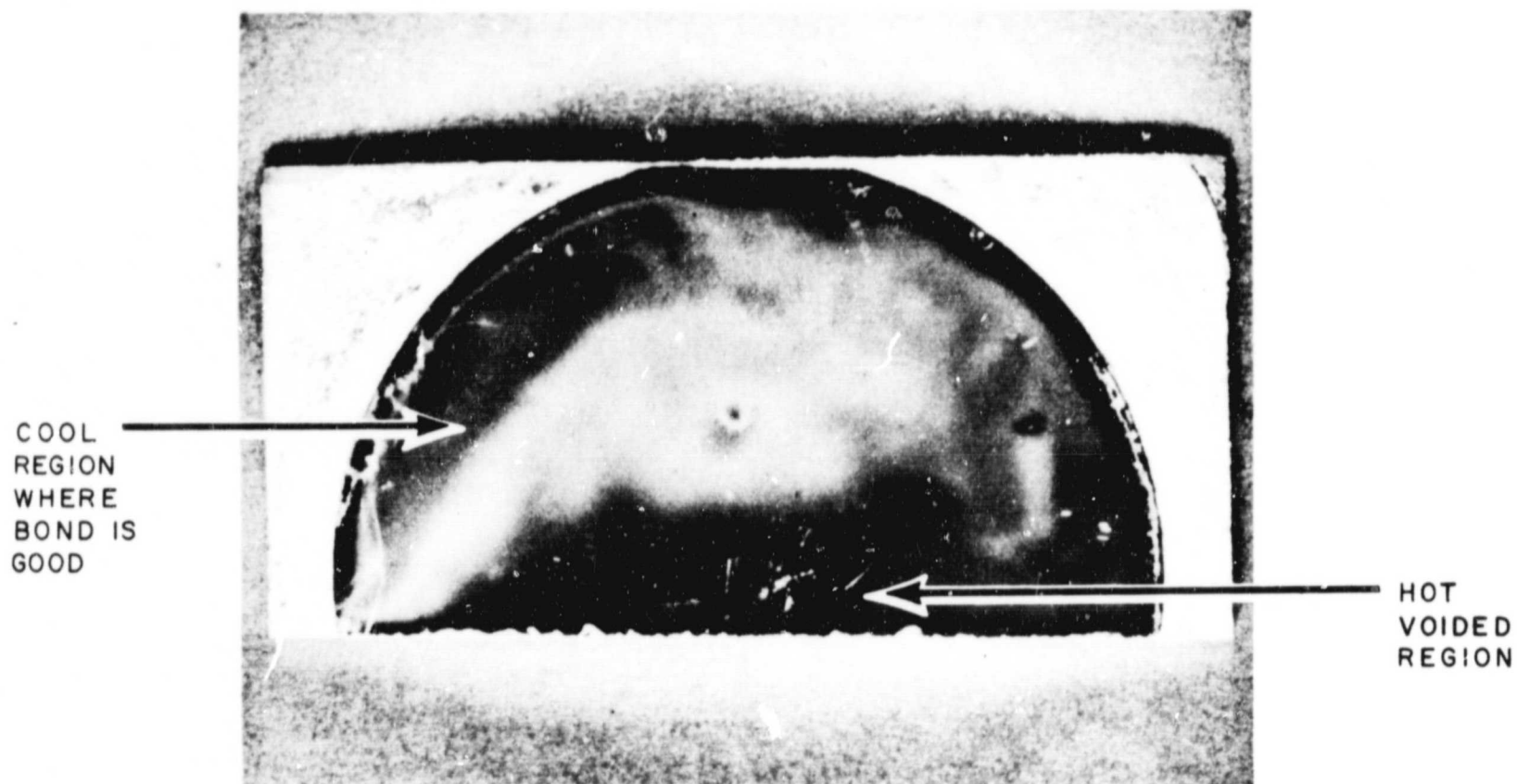


Figure 12. Thermal Patterns Observed Using Liquid Crystal Testing

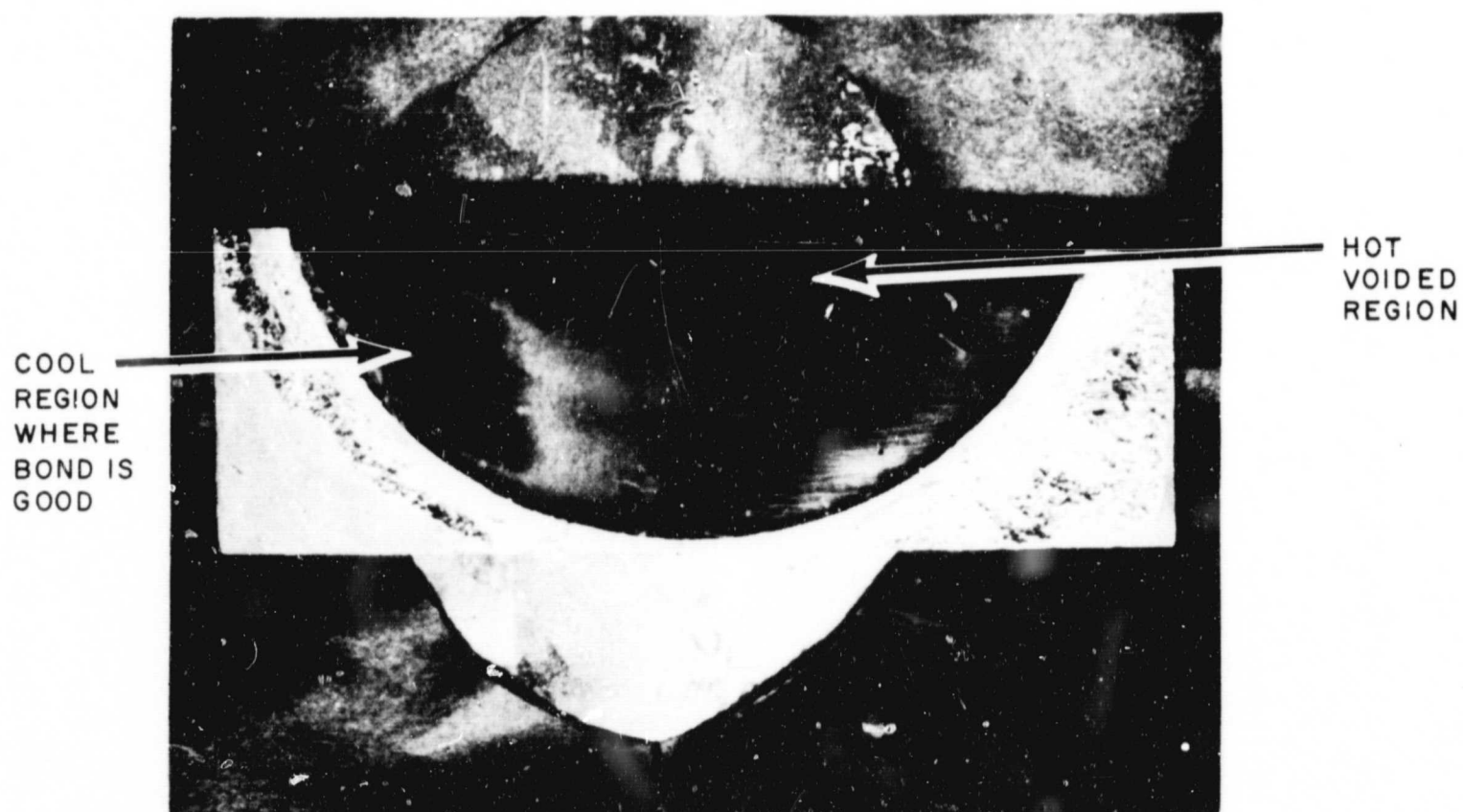


Figure 13. Thermal Patterns Observed Using Liquid Crystal Testing

using five minute anneals at each temperature extreme with five minutes at room temperature between each extreme. A mechanical shock was applied after each cycle to check deterioration and liquid crystals were used to inspect for cracks and new voids. In every case using the Pb-Sn-In, Pb-Sn-In-Cd and pure Sn preforms, the bonds survived more than 10 cycles showing no deleterious effects. In one case where pure In was used, mechanical shock caused the wafer to pop off after the fourth cycle. Close inspection revealed a very lumpy solder layer indicating many voids and therefore a weak bond.

In summary then, the liquid state diffusion bond is very useful if proper precautions are taken to eliminate voids and insure uniform alloying. Although this investigation was almost exclusively confined to the gold-based systems, it seems that silver-based ones provide as much promise in that they will alloy to even higher temperatures. More work is required, however, to evaluate the possibilities of this bonding method.

2.2 SOLID STATE DIFFUSION BONDS

The possibility of the formation of mechanically weak intermetallics when using the liquid-solid type of diffusion bond has led to the investigation of solid-solid diffusion bonding systems. These may be homo- or heterobonds between metals possessing relatively high self-diffusion or interdiffusion coefficients. Homodiffusion bonds are most attractive since there is no possibility for the formation of undesirable intermetallics; however, binary systems do exist wherein near ideal solid solutions form over a wide range of compositions, and where the interdiffusion coefficients are relatively high. One such system which has found use in the vacuum industry for making low temperature brazes is Cu-Au. The phase diagram is given in Figure 14. This is actually a eutectic system, but in the temperature

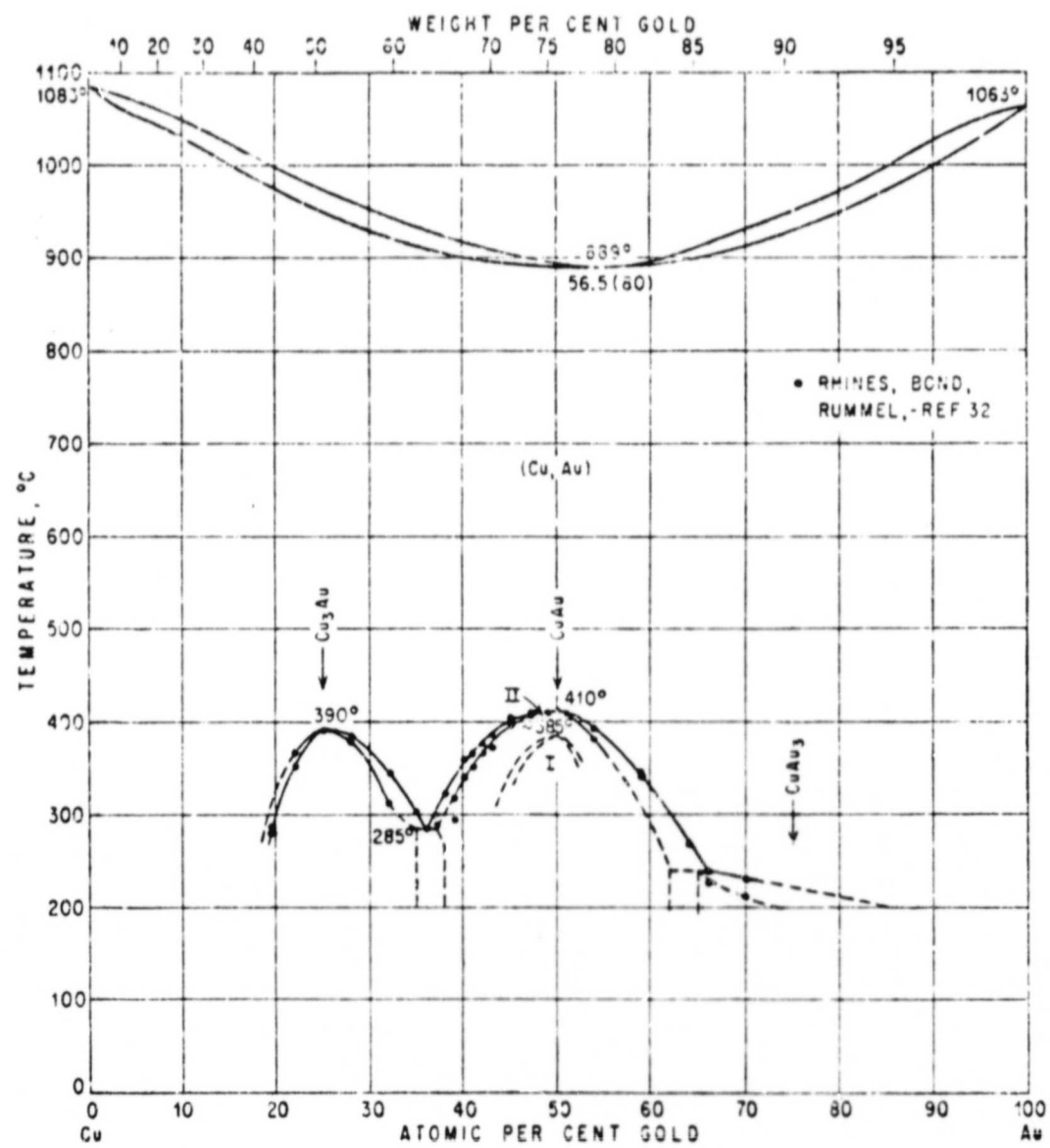


Figure 14. Phase Diagram for Cu-Au

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range where this bonding is done (near 300°C) there exists a uniform single phase solid with some ordering. An even more desirable alternate is the Ag-Au system which is truly ideal and which forms a solid solution at every composition. The phase diagram is shown in Figure 15.

When a diffusion bond is made by this method, it is simply a matter of placing the substrate and wafer in contact and heating it under pressure. In this case, however, the wafer or substrate is not plated with a low melting point material and the only mechanism controlling the process is solid state diffusion.

2.2.1 Bonding Procedures

Substrates and wafers were prepared in a manner identical to the liquid state bonding, except that the low temperature metal was either left out (homogeneous Au-Au bond) or was replaced by a layer of electroplated Ag or Cu. Because of a voiding problem (discussed below), the plated layers on the backside of the wafer were either polished flat or replaced with a Cr-Au metallization developed at Motorola. This consists of the sequential evaporation of 1000 Å of Cr and 10,000 Å of Au on the backside of an etched silicon wafer. The resultant layers are exceptionally smooth and flat. The plated layer on the substrate is lapped on fine diamond paste until a smooth, flat surface is present. For a homo-solid bond, the polished gold surface is used unplated; for a heterobond a layer of either Ag or Cu is evaporated on this polished surface. The substrate and wafer are then clamped under pressure and held at 300°C for 16 to 24 hours. This time is sufficient for complete reaction, and the initial interface disappears.

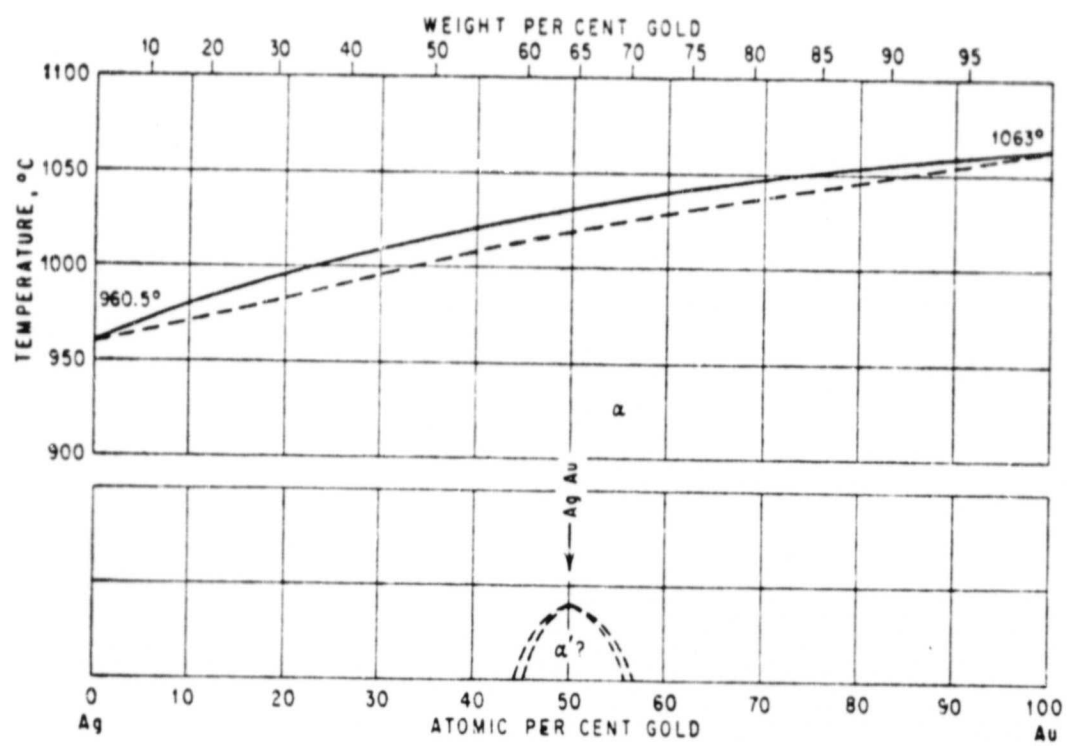


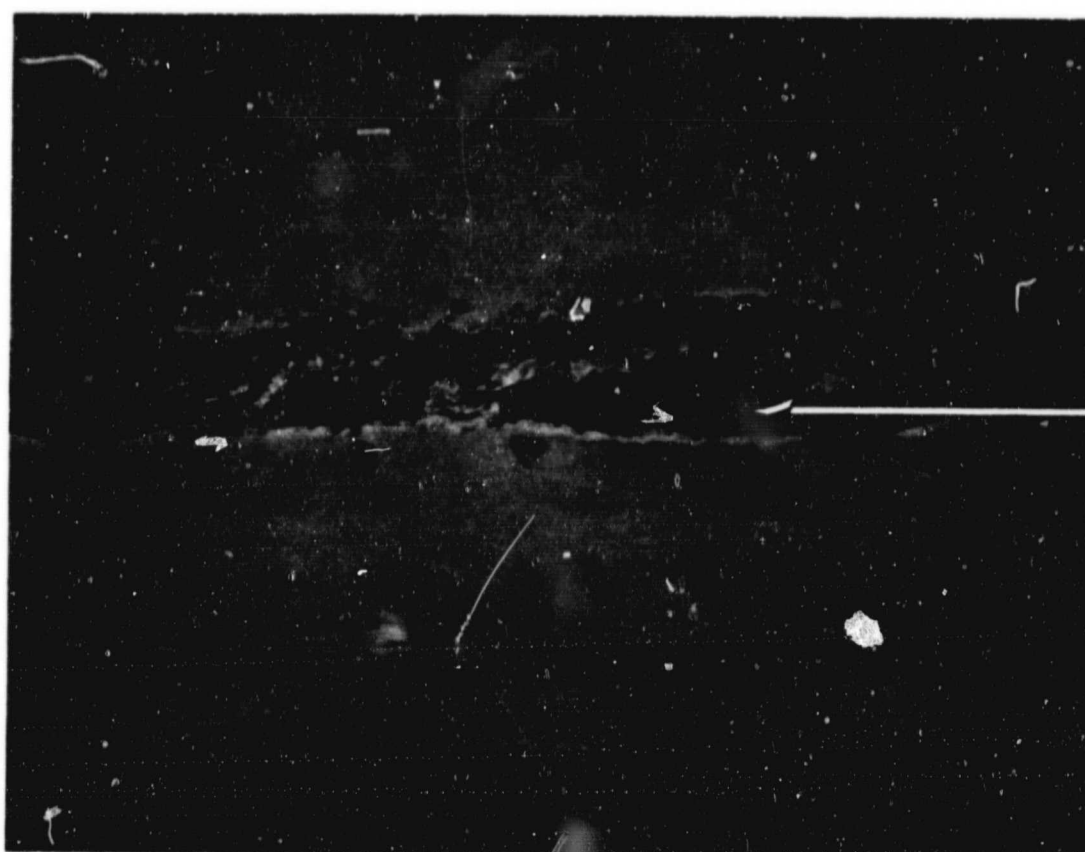
Figure 15. Silver-Gold Constitution Diagram

2.2.2 Problems Associated with Solid State Bonds

Again, the problem of major consequence in making solid state diffusion bonds, is voids. The characteristics of the voids obtained with solid-solid bonds are different than those when a liquid layer is present. For example, even though outgassing of the solid layer occurs, there is no bubble formation with the probability of gas escape being much greater. The problems of the Kirkendall effect, quenching and clustering and chemical reactions with N_2 and H_2 are probably minimal, since in these bonds the anneal temperature is much lower than the solidus of either metal. There are, however, two major effects which may be responsible for poor quality solid-state bonds.

(1) Surface Roughness- Electroplated gold and silver surfaces have a "matte" finish. This means that on a small scale there exist many hills and valleys rather than a smooth planar surface. When the contact area for bonding is small, moderate clamping forces produce pressures great enough to deform the gold and silver into one another and void-free bonding interfaces are observed. (This is the principle underlying the standard thermocompression bond.) When a large area device is bonded (the same clamping system is used), the pressures at contact are greatly reduced, deformation does not occur and cross-section examination of the bonds reveal voids with irregular walls lying along the initial interface (Figure 16).

(2) Uneven Plating- In the plating systems used, the wafers were simply held in a flat-nosed alligator clip while immersed in the various plating baths. In this configuration the density of electric field lines- and hence the rate of metallic deposition -is greatest at the edge of the wafer. The result is a plate which is concave rather than planar. When such a surface is placed in contact with either a plane or another concave one, adherence can only occur at the highest points (i.e., the edges). This phenomenon has been observed



CONTACT VOID

Figure 16. Voids due to Surface Roughness in
Solid-Solid Diffusion Bonds

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with 1.5- and 2-inch diameter silicon wafer-wafer bonds that have been sectioned as a long cigar-shaped void running the entire length of the bond [Figures 17(a) and 17(b)].

2.2.3 Results

A brief calculation of the forces necessary to deform one entire two-inch surface of gold into another, shows that these are impossibly high and hence any hope of using a large scale thermo-compression bond is useless. However, one can simultaneously eliminate both the roughness and the concavity by repolishing the wafer and heat sink after electroplating them with gold. If this is done on fine diamond paste or an alumina slurry, the mating surfaces of the wafer and heat sink are both flat and smooth.

Several homogeneous Au-Au bonds have been attempted at 300°C for times up to 48 hours. In some cases reasonable bonds can be achieved using high clamping forces. However, for the most part the interface seems to remain.

If, on the other hand, a layer of Ag or Cu (1-micron thick) is evaporated on one of the polished surfaces just before clamping and heating, (a forming gas atmosphere must be used), a good bond can be made especially in the case of one wafer to another. Figures 18 and 19 show two such wafer-wafer bonds for the Au-Ag-Au and the Au-Cu-Au system, respectively. These bonds have been made with polished electroplated layers. The total bond thickness is ~0.25 mil and each can be seen to be uniformly alloyed and void-free. Since both binary systems are near ideal, it is expected that both the thermal and electrical resistances of the bonds are quite low. Similar bonds are made using the Cr-Au backed wafers.

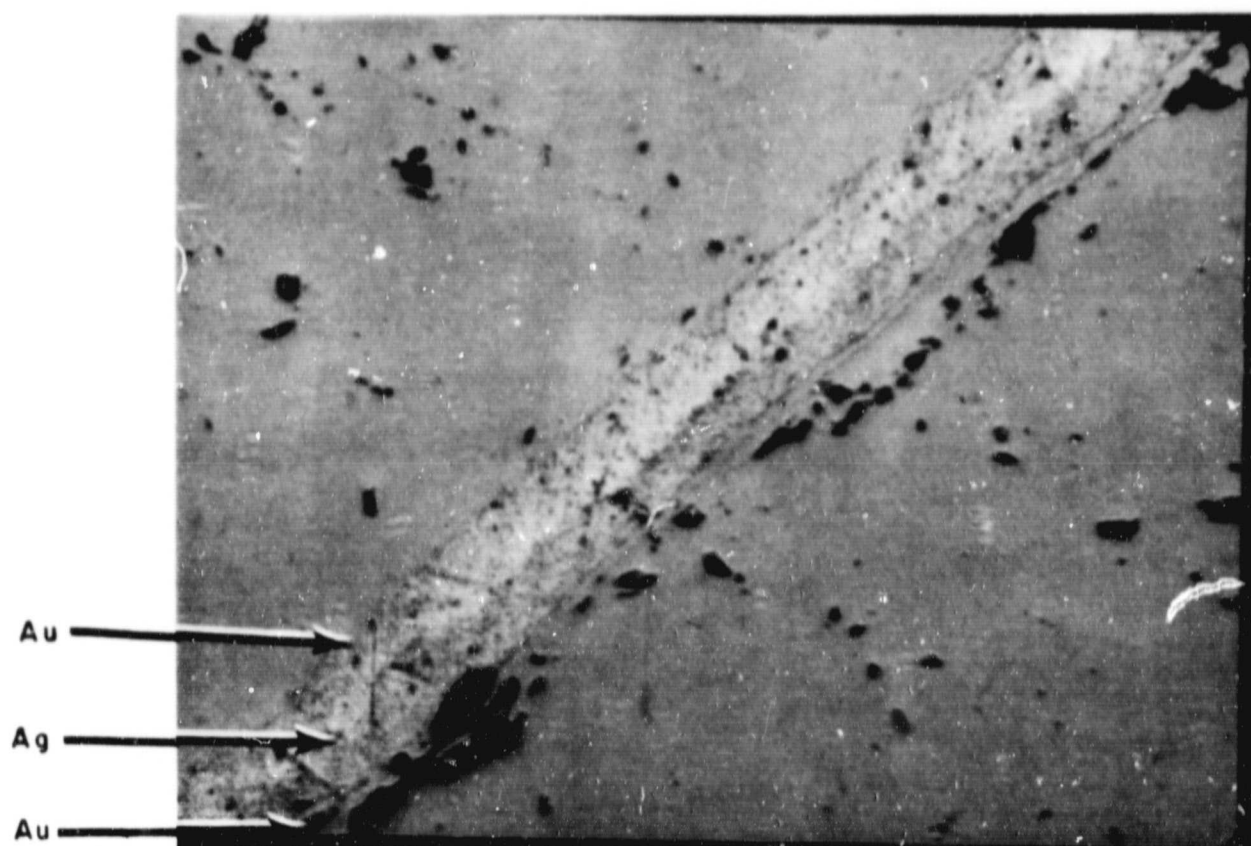


Figure 17(a). Complete Void Free Bond Near Edge of 1.5-inch Wafer (Au-Ag)

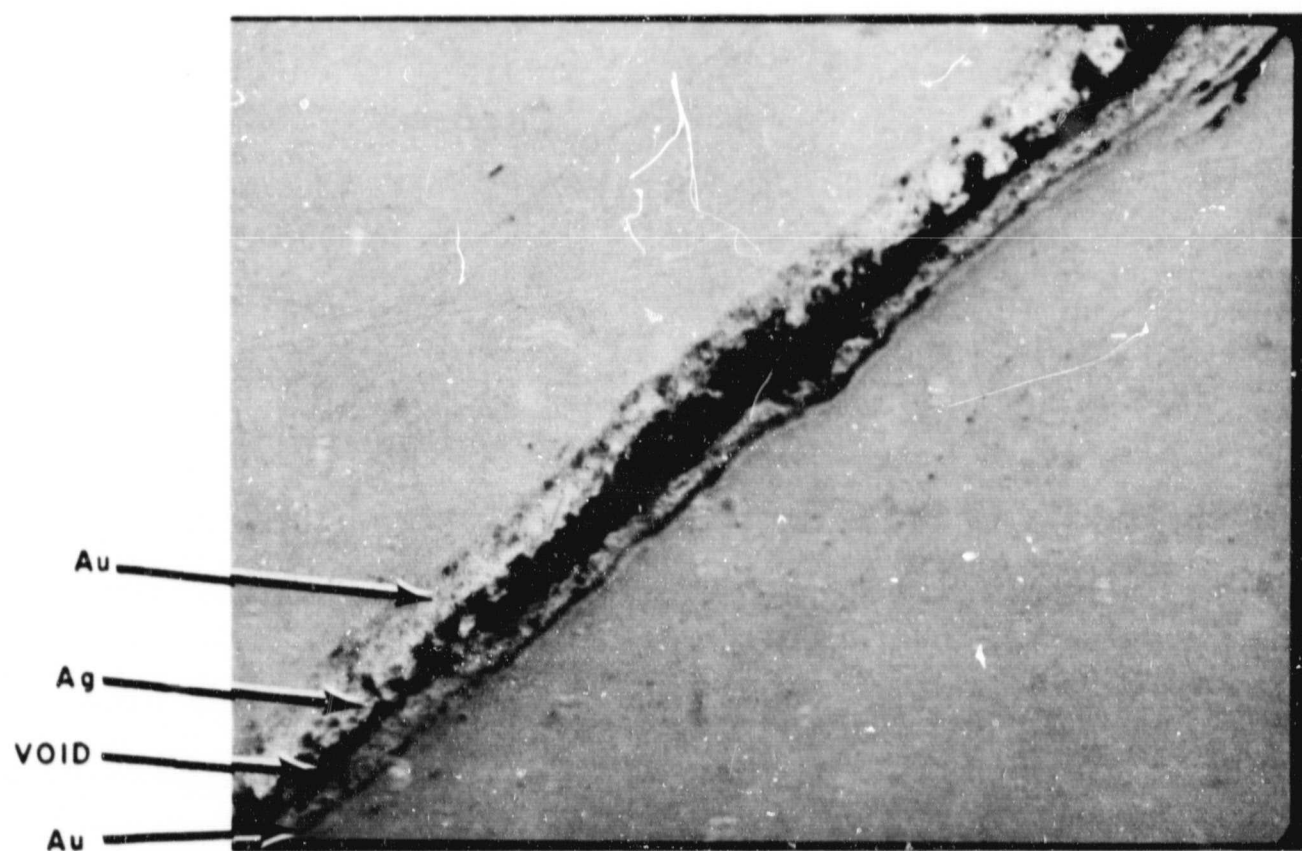
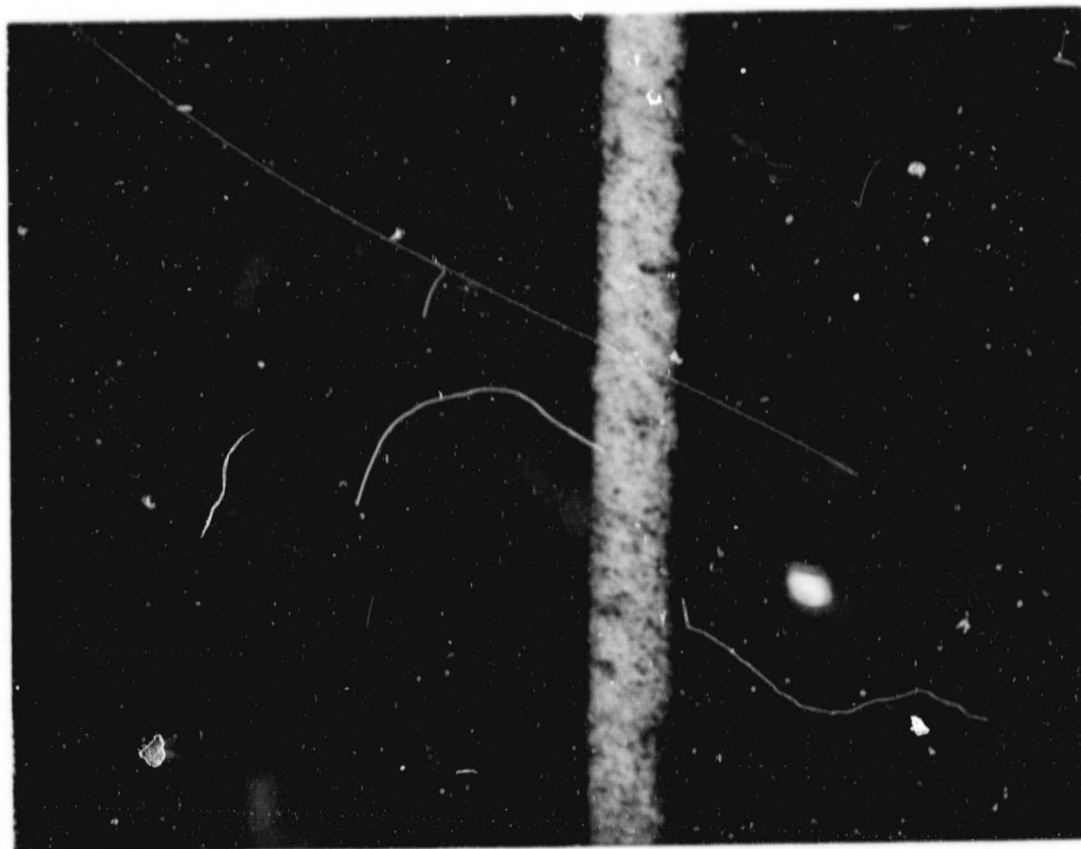
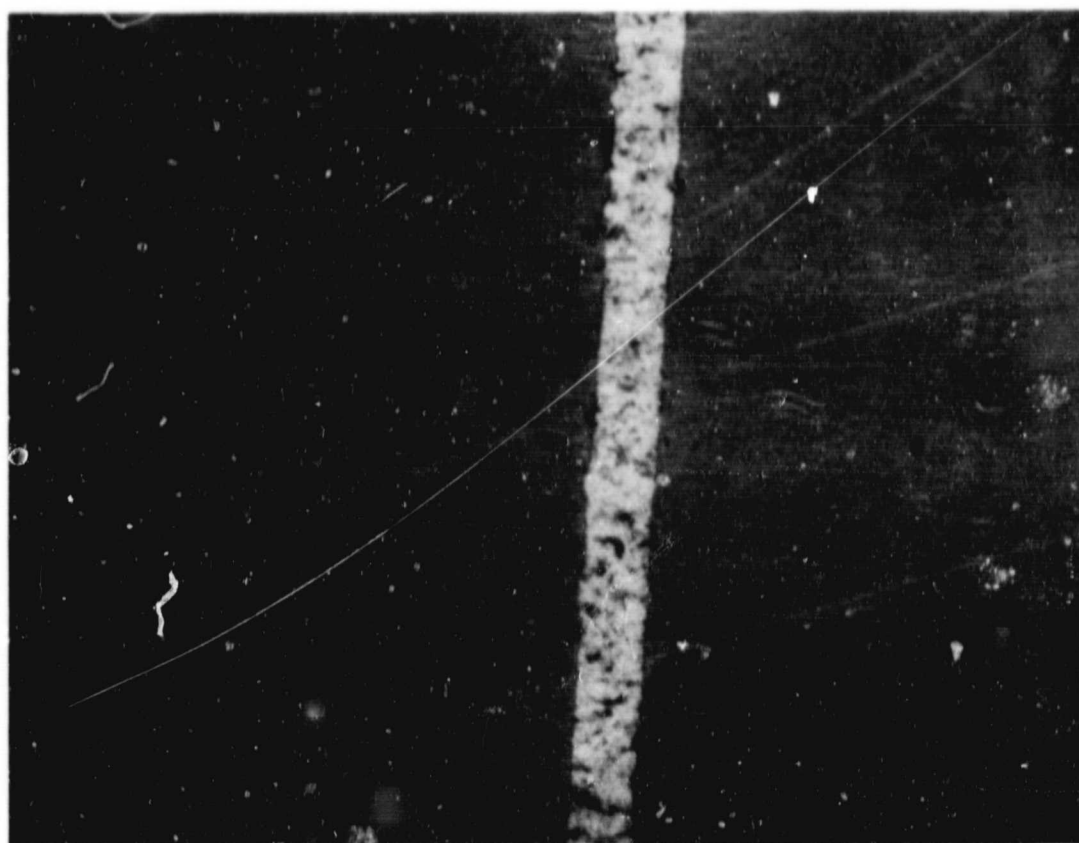


Figure 17(b). Voided Region Near Center of 1.5-inch Wafer Bond (Au-Ag)



1000X

Figure 18. Cross Section Through a Au-Ag-Au
Solid-Solid Diffusion Bond



1000X

Figure 19. Cross Section Through a Au-Cu-Au
Solid-Solid Diffusion Bond

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Liquid crystals have also been used on these wafer-wafer bonds and they show them to be very uniform and having no detectable voids as shown in the cross section.

An unexpected problem has arisen with the wafer-heat sink solid state bond. In almost every case where a wafer one inch or greater is bonded down at reasonable pressures to a heat sink, liquid crystal analysis shows the central region to be unbonded while the edges remain pinned down. Several wafers were etch-cut into dice to verify this. Dice near the edges were well bonded while the central ones could be easily peeled away. Perhaps this can be attributed to a mismatch in expansion coefficient coupled with insufficient interdiffusion of the surface layers. If this is true, then buckling of the wafer upon cooling could destroy the bond near the center. At present no immediate solution to this problem is expected.

An exception to this problem is the case where a wafer is simultaneously heat-sunk on both sides (e.g., Zener diode). In this situation, both bonds can be made with high reliability and the effects on device performance are relatively small. Several large area Zener diodes (1-inch diameter) were bonded using this method. Reverse bias tests showed them to be slightly degraded - a problem which was traced to surface cleanliness rather than poor bonding. Subsequent sectioning revealed bond quality similar to that already shown in Figure 18.

Although the solid state scheme has yielded excellent bond quality for wafers to wafers and the double heat sink, the drawback of extended time for the process and the single heat sink difficulty with large area wafers discussed above indicate the need for future study.

2.3 OTHER BONDING METHODS

2.3.1 Eutectic Solders

The primary method of die bonding to headers involves the use of eutectic solder. The same solder layer results whether preformed and inserted or formed by placing the two base materials together and heating. Examples of such solders are Au-Si, Au-Ge, Al-Si, Al-Ge, Pb-Sn, Au-Sn and a variety of other including ternary eutectic systems. The procedure for making small area die bonds with these solders is commonly known throughout the industry and will not be discussed here. However, certain problems arise when eutectic bonding is employed on a large silicon die. The case of the Au-Si solder typifies these. In a small area bond the silicon die is place in contact with a heated gold layer. The interdiffusion of the materials causes the immediate formation of the eutectic liquid. The die is then "scrubbed" to break up any oxide layers and to remove voids, assuring a uniform bond.

When one applies this scheme to a large area bond several problems arise. First, the scrubbing process is not feasible and hence many voided regions remain under the bond. Secondly, the alloying requires more time and is usually very nonuniform. Thirdly and most significant, the expansion coefficient of these eutectic solders is quite high (See Section 2.4). This is complicated by the fact that since they incorporate some of the substrate material in them they adhere very well and are also very hard. As a consequence

of this, and the fact that relatively high temperatures are necessary to form them, the wafers are severely stressed upon cooling after the bonding process. (This problem with Au-Sn eutectics has been recognized in the industry as the cause of microscopic cracks in dice). This stress usually results in wafer cracking, buckling, or simply tearing the plating loose from the substrate. Systems investigated during this program include Au-Sn and Au-Si. Although the investigations were by no means complete, results were disappointing and no success at applying these high temperature eutectic techniques can be reported.

2.3.2 Amalgam Bonding with Low Temperature Solders

In liquid state diffusion bonding, alloying takes place along an interface between a liquid and a solid layer until, at the anneal temperature, the entire bond volume is solid. An alternate method by which one can obtain a high temperature material is to disperse particles of high melting point materials in a background of liquid metal just before bonding. (This is the principle used to make a dental filling). By annealing at moderate temperatures, then, the solid is dissolved in the liquid until, as in diffusion bonding, the solidus line of the solution is crossed and the amalgam becomes solid.

Several wafer-wafer bonds have been made using an alloy of Ga, In, Sn, which is liquid near room temperature, as the solder, and silver powder as the disperant. One such bond is shown in Figure 20. The bond is void free, but in this case incomplete alloying has left some silver undissolved.

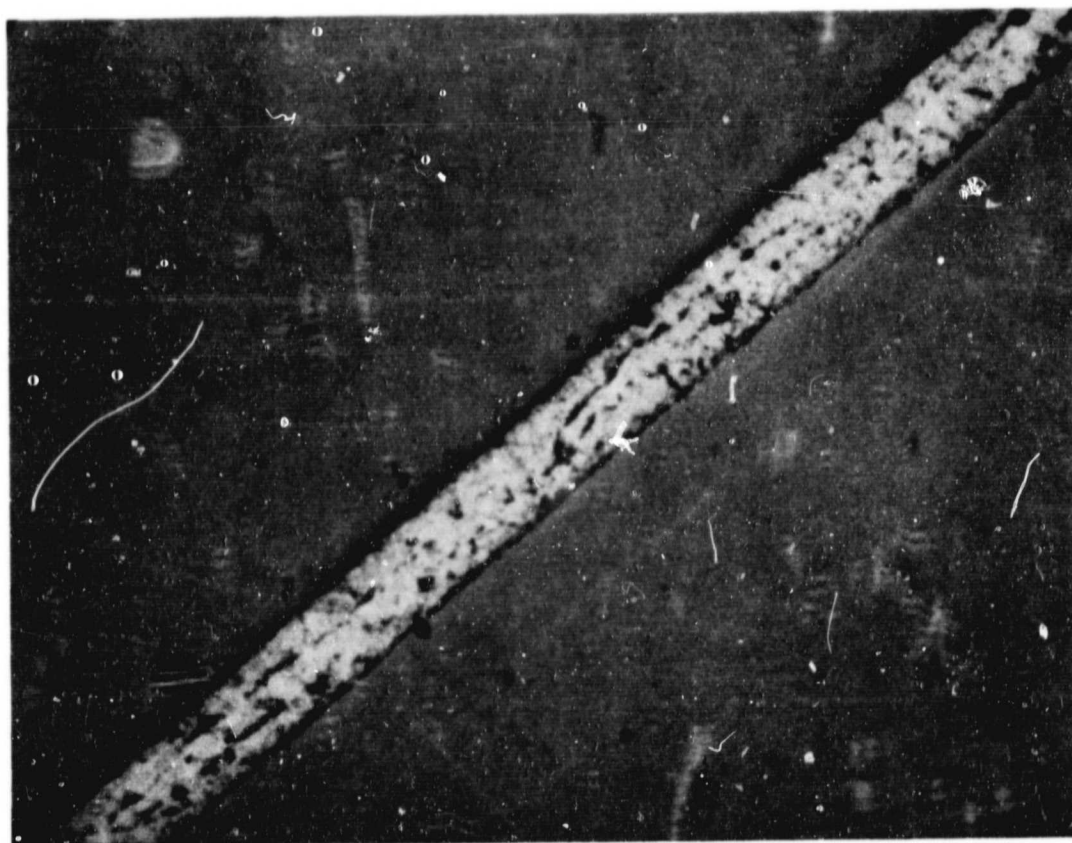


Figure 20. Cross Section of Ga-In-Sn + Ag
Amalgam Bond

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Melting point tests show that the solder remains solid to about 350° even though the bonding temperature was below 200°C.

It is apparent that this method shows promise although much is to be learned about the technique of making such bonds. The large surface-to-volume ratio of the dispersed powder appears to decrease the anneal time from what it would be if the system were layered. However, it must be remembered that since these solders are liquid near room temperature or slightly above, more high temperature material and longer anneal times may be required for alloying to form a solder operating at the temperatures dictated by electronic systems.

2.3.3 Filled Epoxy Bonds

In recent years great advances have been made in organic binders. The commonly used "epoxy" glues are among them. Some published data indicate that when such materials are "filled" with metals of high thermal conductivity, the thermal conductivity of the mixture is enhanced while the adhesive properties are not substantially affected. Data⁽³⁾ using aluminum powder, aluminum wool and various carbon mixtures indicate that at filler concentrations greater than 80 percent by weight, the thermal conductivity is not very much lower than many eutectic solders. It would seem then that if these easily applied materials can be utilized for large area bonding, a simple yet effective bonding scheme could result.

During this contract period one such filled epoxy resin was investigated, "Eccobond 99" a product of Emerson and Cummings, Inc. This non-flowing paste which is spread on with a spatula, is black in color, soluble in standard organic solvents such as TCE and toluene, has almost unlimited shelf-life if refrigerated, and cures in one hour at 150°C. It has a thermal conductivity claimed to be 4×10^{-4} cal-cm/cm²-sec-°C (we have measured this as 3×10^{-4} cal-cm/cm²-sec-°C) which is significantly lower than any metal solders which we have employed. Its thermal coefficient of expansion when cured is about 35 ppm/°C.

Although many one-inch wafer bonds were made to various heat sinks, none was much of a success for two reasons. First, the epoxy shrinks a great deal when curing; this causes an enormous amount of wafer buckling and cracking. Secondly, in order to assure a void free bond, all trapped gas must be removed from the epoxy layer before curing. This requires outgassing under vacuum, a step which is both time-consuming and expensive. Even if this could be done it seems that the use of filled epoxy binders, particularly the system discussed here, is not practical.

2.3.4 Anodic Bonding

In many industrial journals over the past few months, there have appeared articles describing a new bonding process. This so-called anodic bonding⁽⁴⁾ is especially useful for bonding metals (particularly semiconductors) to glass and other glass-like materials. The process makes use of temperature and electric fields to bond the two materials together; no solder,

adhesive or other bonding material is necessary. Furthermore, the bonding is made to a material which can be matched in expansion coefficient to the silicon, and the thermal excursions, even though they are relatively small, are easily tolerated. In no case is the bond heated to the softening point of either material.

In the particular setup used for evaluating this process at Motorola, the bonding was done on a carbon strip heated with regulated alternating current. In addition to the heating function, the strip was made the positive electrode of the dc system. A schematic of the bonding system is given in Figure 21.

To make a bond between silicon and glass, Pyrex for example, one simply assembles the system as shown, heats it up to 500°C (this temperature is typical for pyrex although bonds have been made as low as 400°C), and then applies 400 to 500 volts dc. No special atmosphere is required. A small current flows (1 to 4 microamperes), and as the bond is made, one observes white light interference fringes disappearing until intimate contact is complete. Further time at temperature and voltage does not appear to effect the bond quality.

Many bonds have been made with 0.5-inch and 1-1/4-inch wafers to Pyrex glass substrates. A cross section of such a bond is shown in Figure 22. It can be seen that the bonds are extremely uniform and completely void-free. The bonds are also as strong as they look. When attempts were made to break a bond, either the glass strength limited the bond quality or the silicon sheared. In no cases did the bonded interface account for the weak part of the system.

The obvious drawback of this system is the use of glass as a substrate material. Glasses are notoriously poor thermal

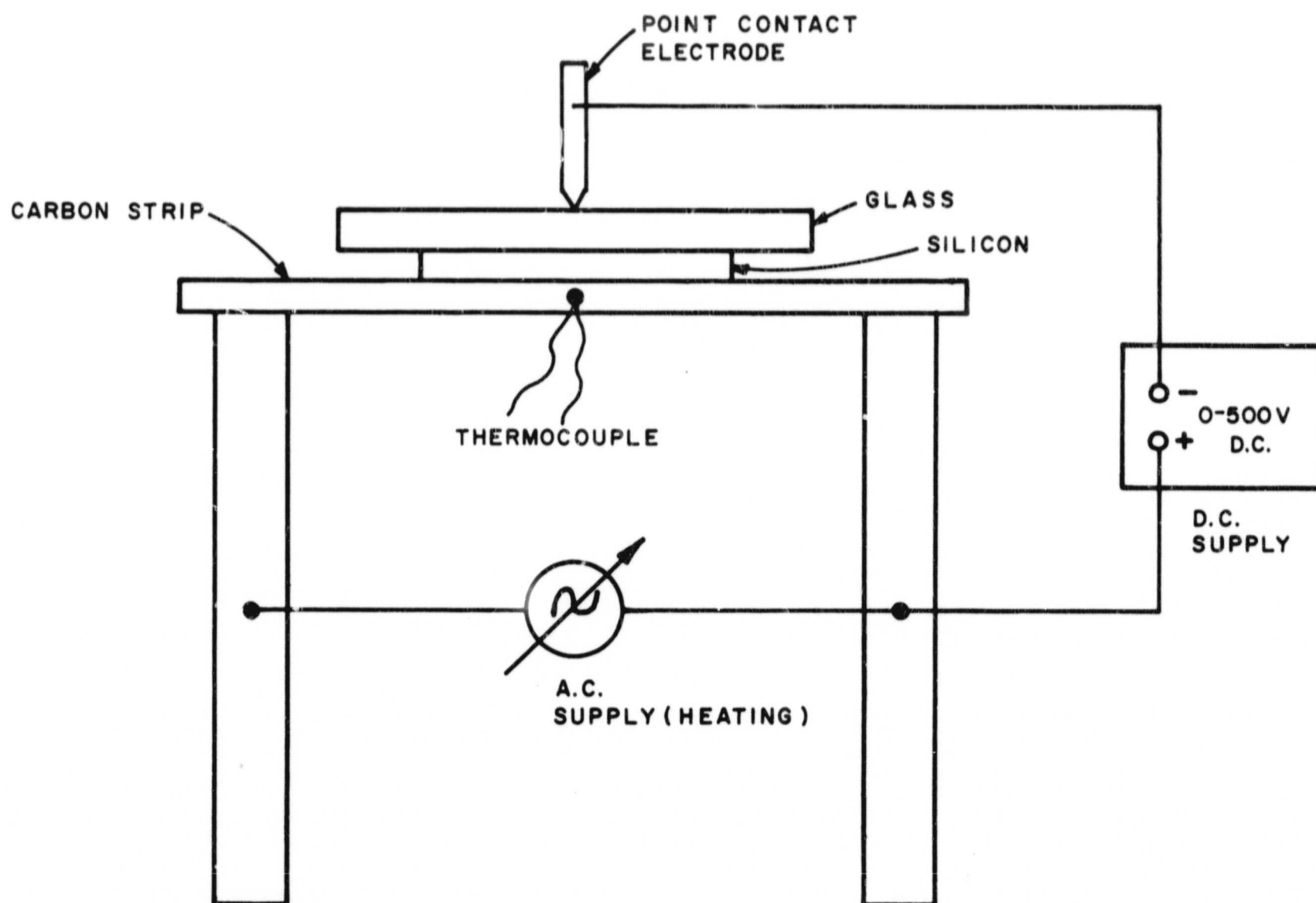


Figure 21. Schematic of Anodic Bonding Apparatus

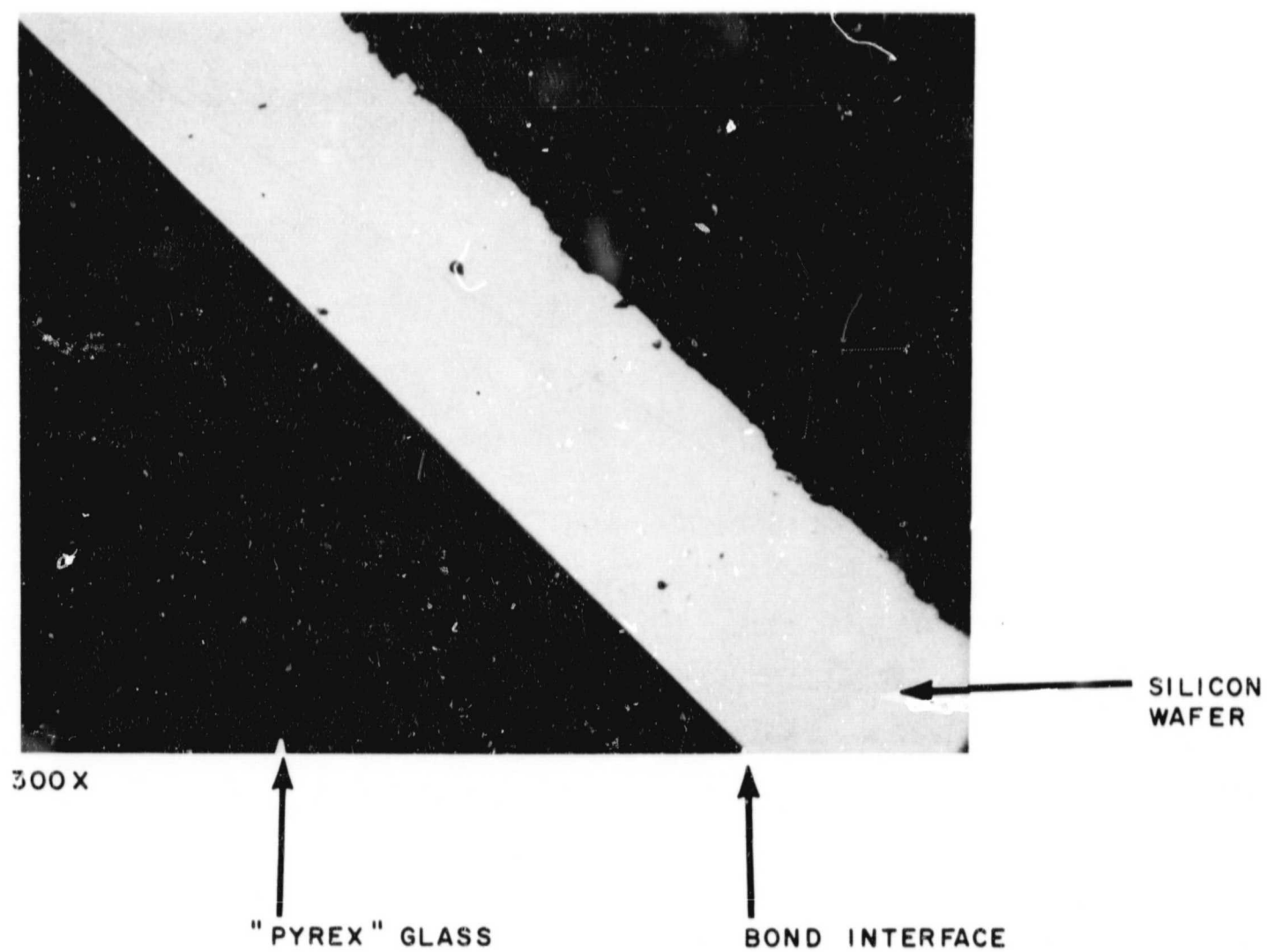


Figure 22. Anodic Bond of Silicon to Glass
500°C 400 V dc

conductors and are generally fragile. However, the process might be employed for bonding large area dice to glazed alumina, beryllia, or metal wherein the effect of the conductivity of the glass layer would be minimized by keeping it thin.

Since this process is so new and appears to be so useful, future research in this area should yield many useful applications.

2.4 THERMOPHYSICAL PROPERTIES

2.4.1 The Eutectic Solders

A large amount of die bonding in the industry today is done with eutectic solders. These are often times mismatched to the job, and a trial and error approach is used in selecting them. This match-up is particularly important when the area of the bond becomes large. A better understanding of the use of eutectic solders can certainly be had if the properties of the individual systems are known. It was with this intent that certain measurements of basic thermal and mechanical properties were undertaken for five solder systems. The particular binary alloys chosen are listed with their melting points in Table III. These systems were chosen because they represent a fair cross section of the commonly used solders of the semiconductor industry and were readily attainable. The specimens were prepared by Alloys Unlimited Inc., of Melville, New York.

2.4.2 Thermal Conductivity

Motorola purchased a thermal conductometer⁽⁵⁾ manufactured by Colora Messtechnik G.m.b.H. of Germany (See Figure 23) to enable an accurate determination (± 3 percent) of the thermal conductivity

TABLE III

Alloy	Composition (wt %)	Melting Point (°C)
Au-Ge	88-12	356
Au-Si	97-3	370
Au-Sn	80-20	280
Al-Si	89-11	577
Pb-Sn	37-63	183

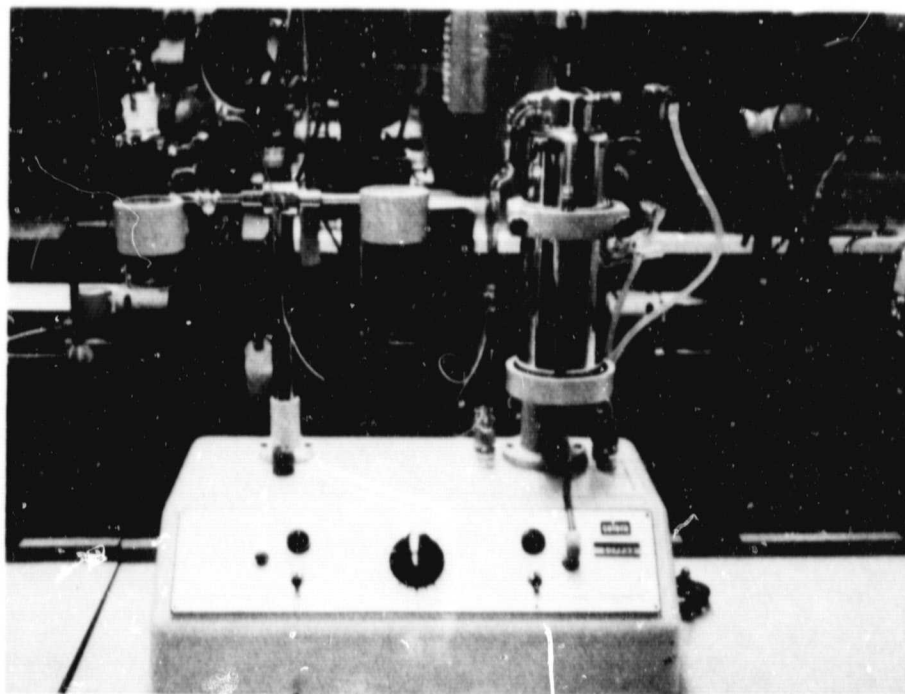


Figure 23. Colora Thermal Conductometer

of potential package materials. The thermal conductometer is based upon a steady state measurement of thermal flow determined by the rate of liquid evaporation due to the thermal flow. The rate of liquid evaporation is compared to a graph which was previously determined by means of calibrated samples.

For these measurements pellets of all five binary eutectic alloys were ordered. These were 0.65 x 1.0 inches and were void free. Our inspection and subsequent sectioning validated this. Three pellets of each solder have been measured a minimum of four times each and the results averaged. All measurements represent conductivity values at 100°C. The conductometer was recalibrated (though no drift could be detected) at least three times throughout the measurements.

Results for the five binary systems are given in Table IV. The conductivities are in standard CGS units, $\text{cal-cm/cm}^2\text{-sec-}^\circ\text{C}$.

TABLE IV
MEASURED THERMAL CONDUCTIVITY
OF SELECTED EUTECTIC SOLDERS

Solder	Conductivity (Cal/cm/sec°C)
Au-Sn (80-20)	0.069
Au-Si (97-3)	0.031
Au-Ge (88-12)	0.060
Al-Si (89-11)	0.196
Pb-Sn (37-63)	0.097

It is difficult to make comparisons to much of the existing data tables for thermal conductivity since in very few of them is the temperature of measurement quoted. This parameter is a

decreasing function of temperature and therefore, we might expect our values (100°C) to deviate from any quoted in the room temperature range and be significantly lower than the values quoted at 4°K and lower. Figure 24 shows a plot of handbook values for various Pb-Sn solders including a point for the alloy we have measured. Since no temperatures are given with the handbook data, a direct comparison may not be justified. However, a slight discrepancy appears to exist.

In addition to the above reasons, it is believed that the conductometer may introduce more error when high conductivity materials are measured. This can be due to a turbulent rather than equilibrium evaporation of the lower vaporization point material.

The fact that the eutectic systems manifest thermal conductivities much lower than the pure metals from which they are made is noteworthy. For example, in the gold-tin system the eutectic conductivity is 0.069, while for Au it is 0.70 and for Sn it is 0.15 where all of these are in CGS units. This is to be expected if one studies the conductivity versus composition curves of various binary systems. The presence of impurity atoms causes perturbations in the lattice structures of the metals and one expects a concurrent decrease in the conductivities.

The fact that these conductivities are so low points to the need for using solders which manifest pure metal properties (solid solutions) at compositions near the ends of the phase diagram. Such solders are possible by the diffusion bonding approaches discussed earlier.

2.4.3 Coefficient of Thermal Expansion

In this phase of the program, the thermal expansion coefficients of the five previously discussed eutectic solders were

Pb-Sn SOLDERS

⊙ LITERATURE VALUES (NO TEMPERATURE GIVEN)

Δ THIS EXPERIMENT (100°C)

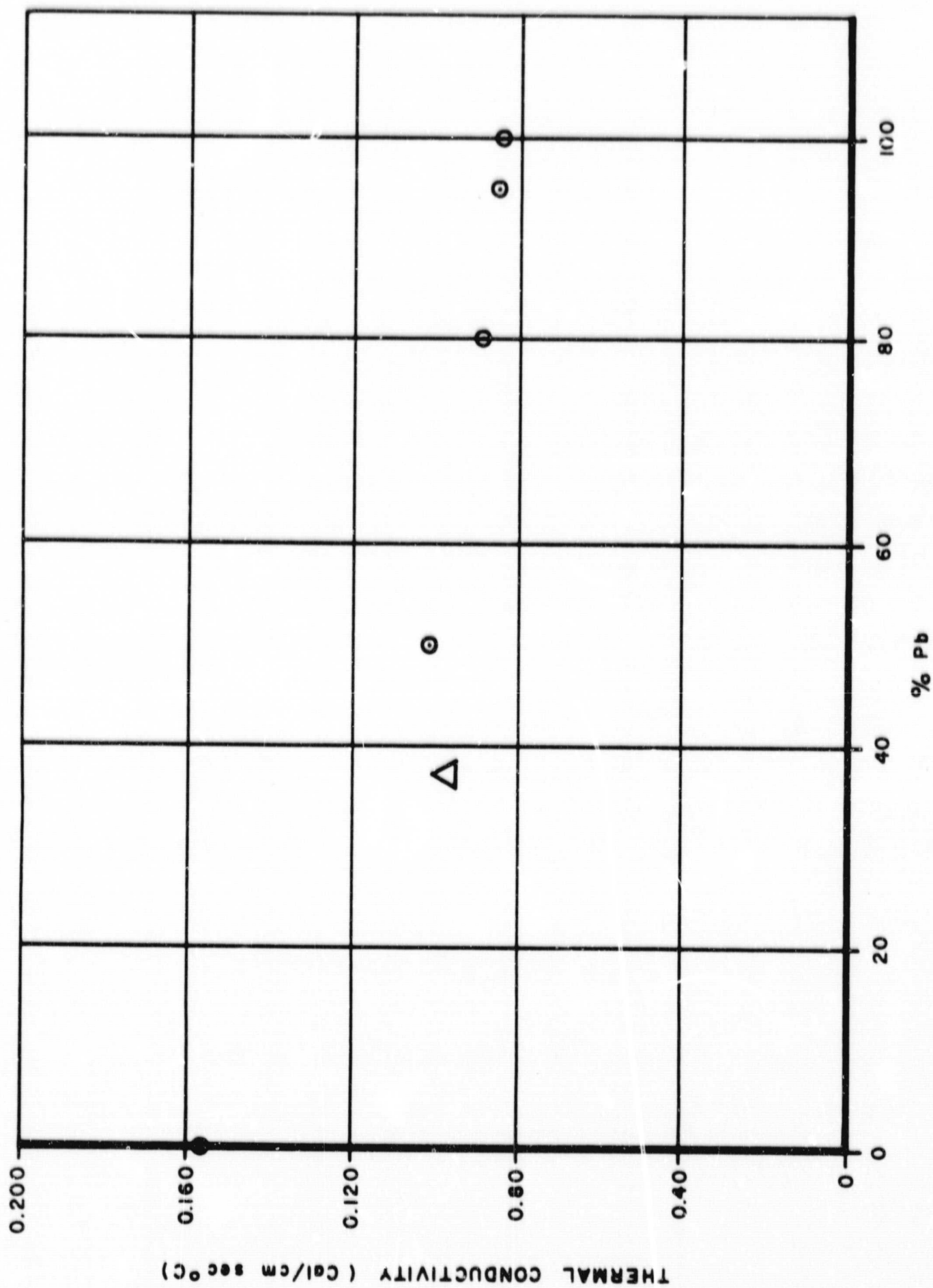


Figure 24. Thermal Conductivity of Common Pb-Sn Solders

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measured. The thermal conductivity samples were machined down to 0.50 x 1.0 inches to accommodate the system used for the measurements.

The apparatus with which the coefficients of expansion were determined consisted of a variable temperature oil bath contained in a 3-necked globe flask, a dial gage and a dilatometer. By using a voltage control device, the temperature of the oil bath could be adjusted to within five centigrade degrees at any level from room temperature to 200°C. Measurement of the bath's temperature was accomplished with a mercury thermometer placed in a stem well which extended into the oil bath. Pump oil with a flash point of 410°C was used for the bath. Expansion measurements were made with a Brown & Sharpe dial gage readable to ± 0.00002 inches. The dilatometer is a quartz tube with a flat seal at one end which holds the specimen snugly inside. A quartz rod, rounded on one end and flat on the other, was fit inside the quartz tube and set atop the sample. The material being tested is trapped at the bottom of the tube between the flat bottom and the rounded end of the rod. When the lower end of the device is submerged in the oil bath, the sample's expansion is transmitted by the rod to the dial gage which is mounted against the rod's flat upper surface. If a graph is constructed of dial gage reading versus sample temperature, the thermal expansion coefficient appears in the slope. This is easily demonstrated by the general formula for thermal expansion:

$$L(T) = L(T_0) [1 + \alpha(T - T_0)]$$

Therefore, the slope of the aforementioned graph is

$$\text{Slope} = \frac{\Delta L}{\Delta T} = \alpha L(T_0)$$

where

$$\Delta L = L(T) - L(T_0) \text{ and } \Delta T = T - T_0$$

The results of the experiments on the five eutectic solder systems are given in Figures 25, 26, 27, 28, and 29; and the expansion coefficients are summarized in Table V.

TABLE V

Solder	α (ppm/°C)
Au-Ge	14.1
Au-Si	14.2
Au-Sn	17.1
Al-Si	23.1
Pb-Sn	22.1

Two of these systems (Au-Sn, Au-Si) have been measured by another method elsewhere⁽⁶⁾ and the present results agree within a few percent. The shapes of the curves, including "kinks" are also in agreement.

The results show that in these systems where there is such a dominance of one component and it forms a contiguous phase, the coefficient of expansion is almost identical to the major constituent. This is a commonplace occurrence in such systems. Furthermore, these results indicate that nothing is to be gained by using eutectic solders to solve expansivity problems. It seems that the only way a better match may be obtained is through the the formation of intermetallic compounds, which may be widely different in expansivity than their parent materials.

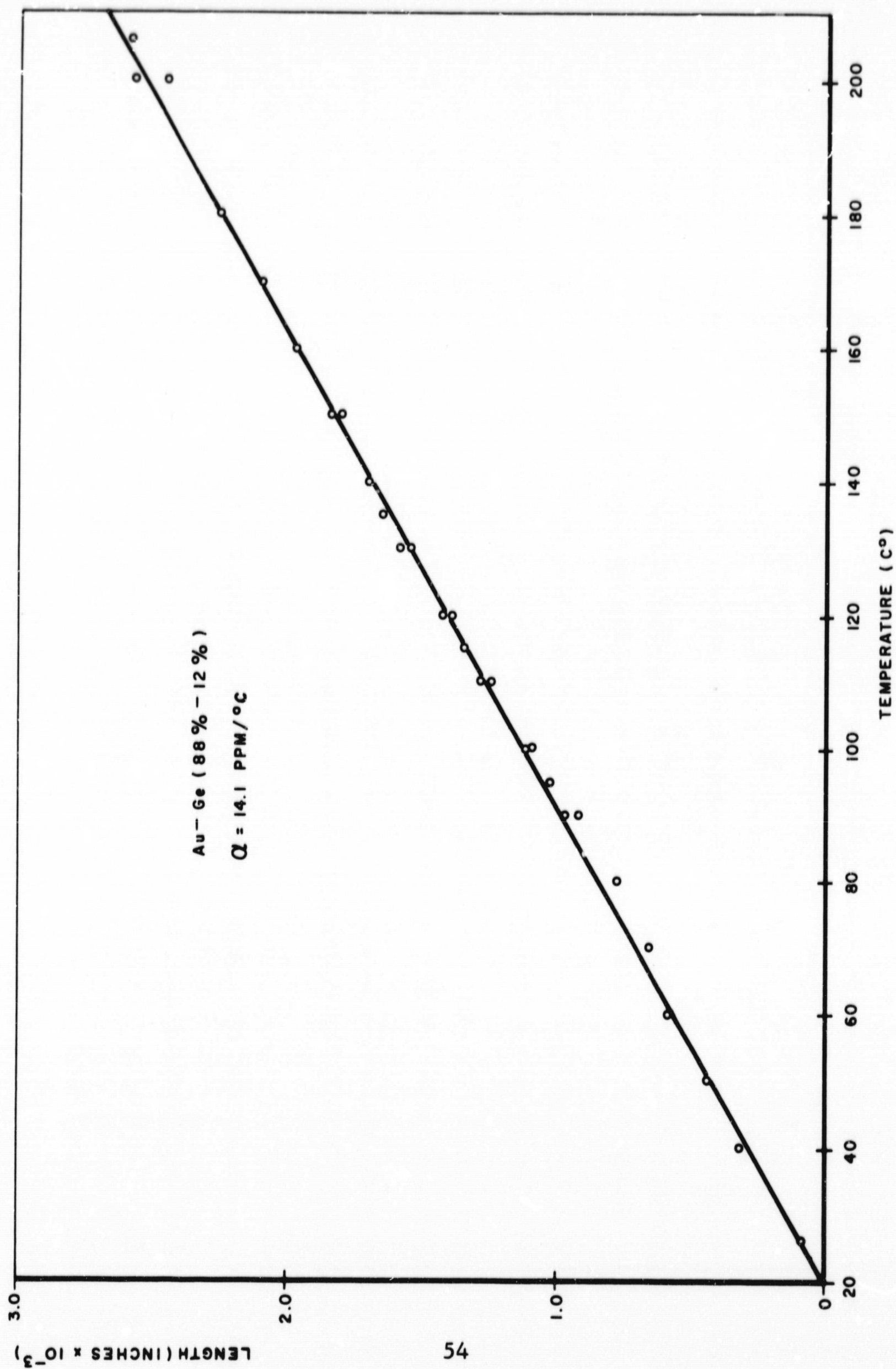


Figure 25. Dilation Curve for Au-Ge

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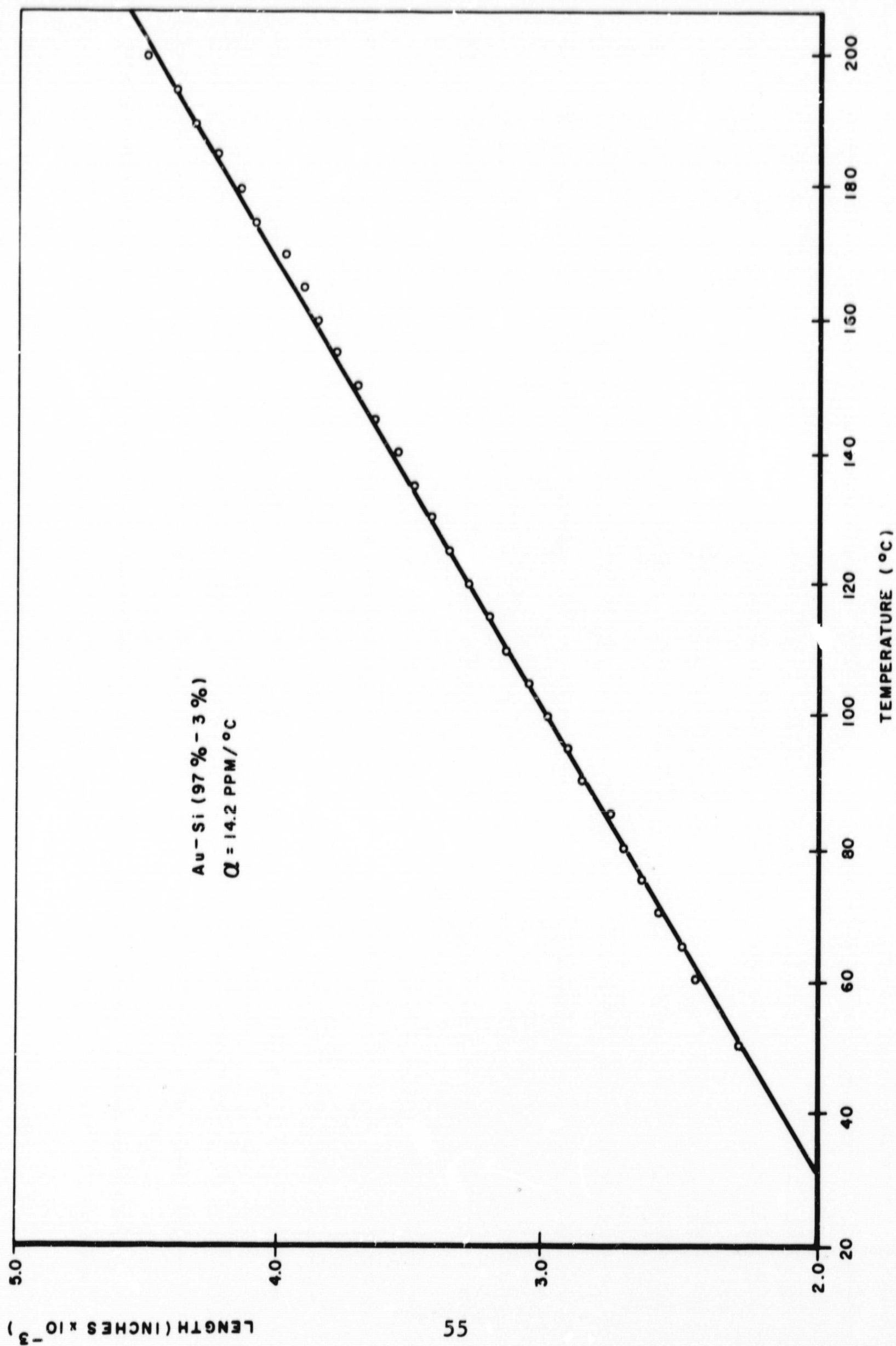


Figure 26. Dilation Curve for Au-Si

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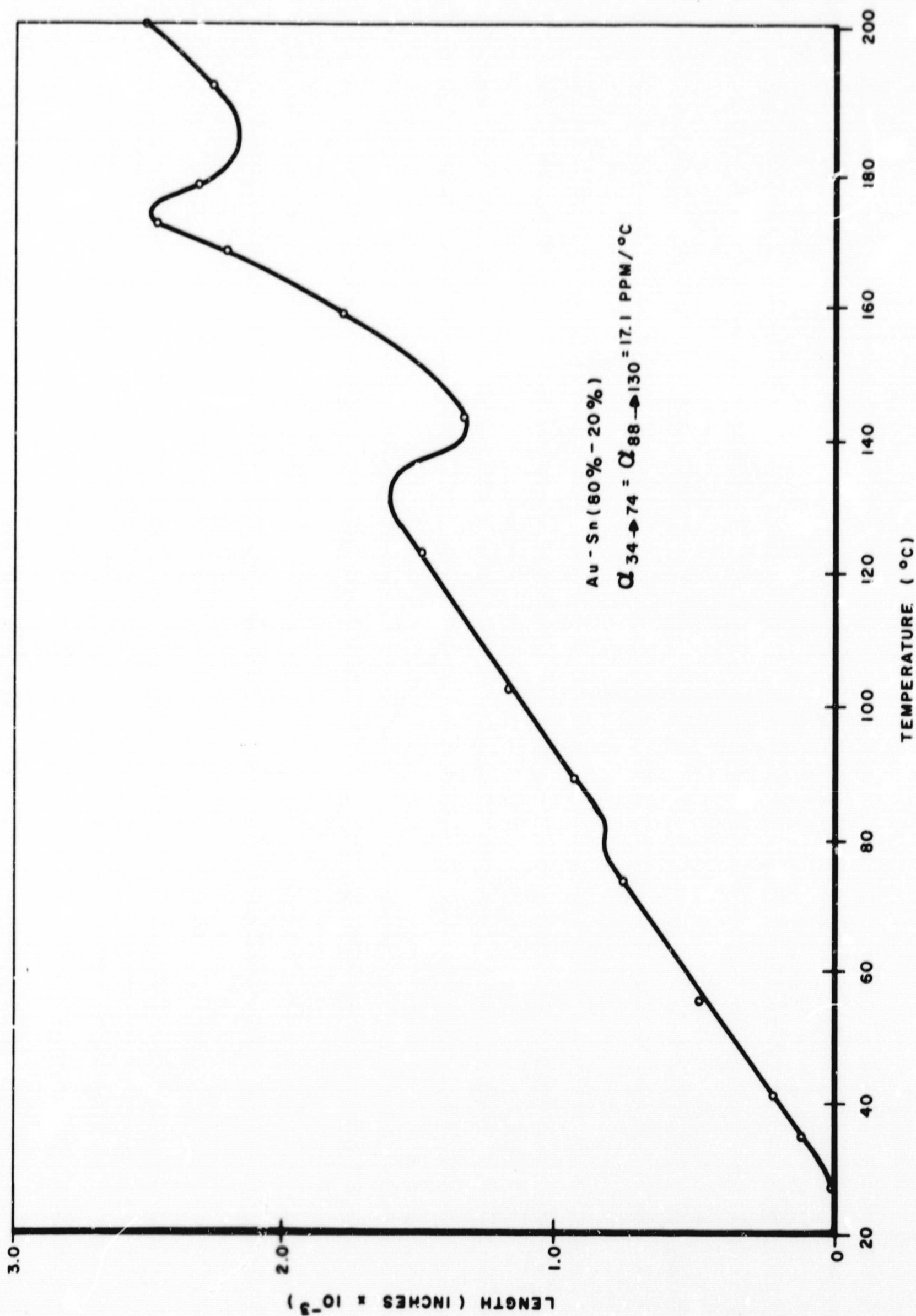


Figure 27. Dilation Curve for Au-Sn

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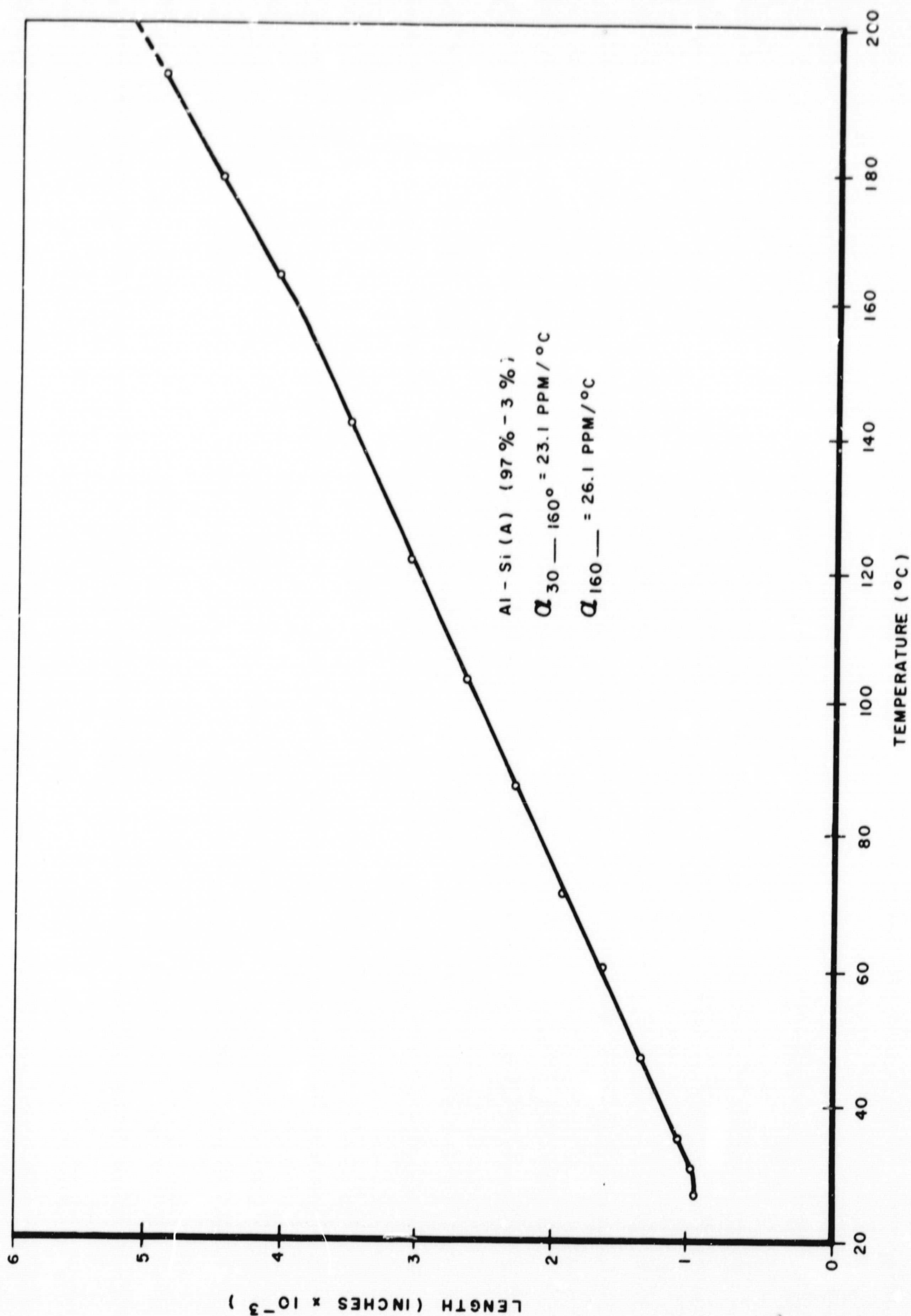


Figure 28. Dilation Curve for Al-Si

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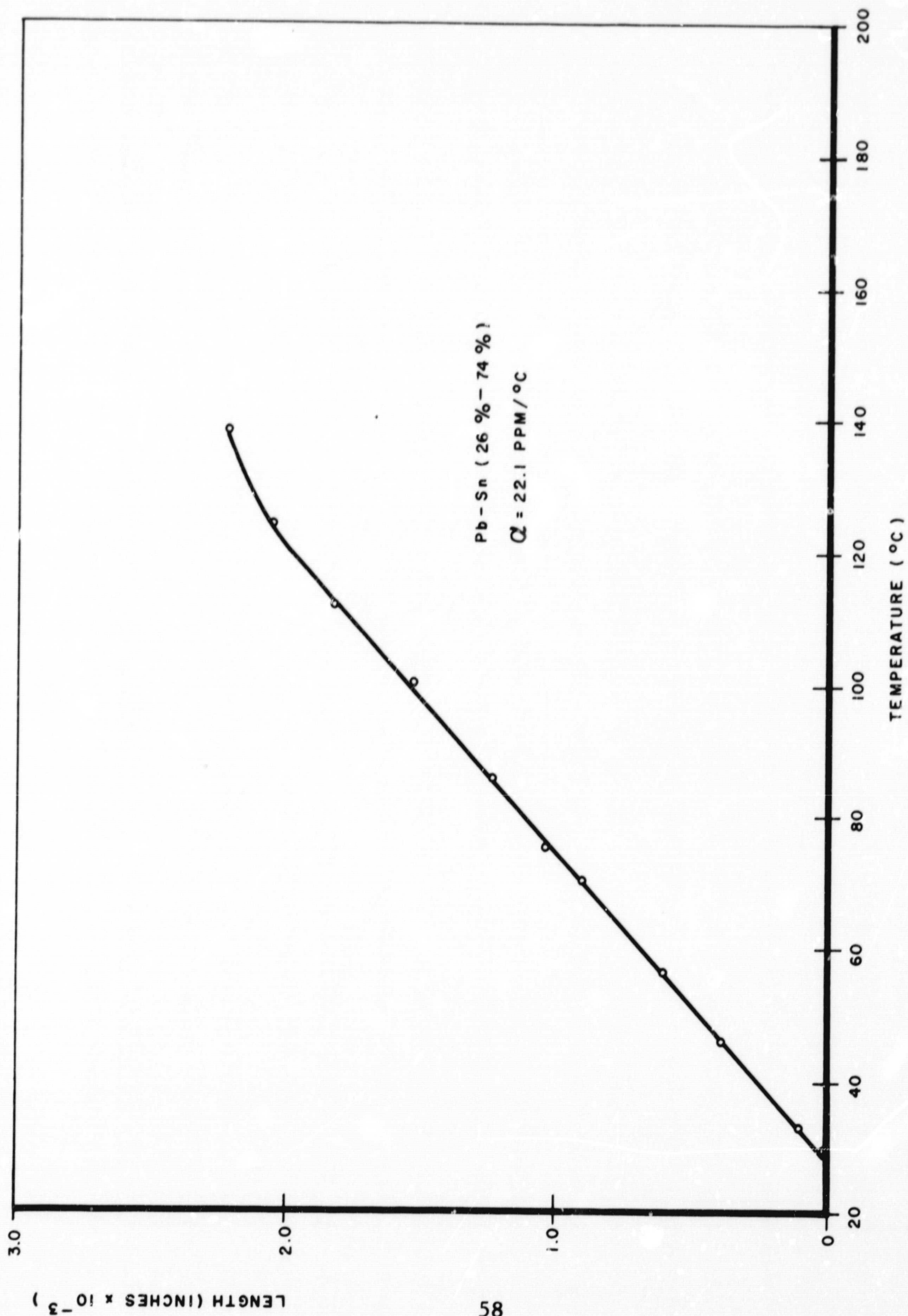


Figure 29. Dilation Curve for Pb-Sn

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2.4.4 Mechanical Properties

Original plans called for measurements of the Elastic Modulus and tensile strength of these systems. Orders were placed with Alloys Unlimited for standard tensile specimens. The estimated degree of difficulty in fabricating these samples was far exceeded because in every case the materials were extremely hard and brittle. Further plans for conducting tensile measurements were abandoned because it was felt that the information which could be obtained (e.g., that these were brittle compounds) would not meet the investment cost in value.

2.4.5 Properties of Silver-Indium

Because most of the effort of this program was devoted to diffusion bonding, and for a further understanding of the typical systems used in this process, an investigation of the properties of a I-III binary system was undertaken. The purpose was to generate engineering data on thermal conductivity, thermal expansion coefficient, elastic modulus and tensile strength for a system from which one could infer properties of other similar metal alloys, which might be formed during a bonding process.

The binary system chosen was Ag-In; the reasons for the choice being threefold:

- (1) It was presumed that the properties of Ag-In were typical of solders formed from the I-III and I-IV groups of the periodic table.
- (2) Materials for fabrication are readily available, easy to work with, and have well-known properties in the pure state.

- (3) Because fabrication of the samples might prove difficult and require relatively large amounts of material, silver was chosen in preference to gold.

2.4.6 Coefficient of Thermal Expansion

The quartz dilatometer described above was used to measure thermal expansivity of the indium solid solution. Values for the silver solid solution have been published⁽⁷⁾. Because of the difficulty in machining the intermetallic compositions, experiments were confined to 20 percent or less of the minor component. Results for the indium and silver solution regions are given in Figures 30 and 31, respectively. Each point is derived from a graph similar to Figure 25 through 29. The curves show no unexpected trends and since the expansivities of Ag and In are 18.7 ppm/°C and 33 ppm/°C respectively, the increase with addition of indium and decrease with addition of silver might be expected. It is noteworthy that these alloys do not have a much better expansion coefficient match to silicon than the eutectic solders. However, since the solid solutions are relatively soft compared to the eutectics, some stress relief is to be expected when they are the interface between a wafer and substrate.

2.4.7 Thermal Conductivity

Using the Colora Thermal Conductometer, previously described, the thermal conductance of several samples selected from across the Ag-In phase diagram was measured. In this case, sample preparation was quite difficult (especially where indium was the major component), and reliable data was forthcoming only in the composition range where silver dominates.

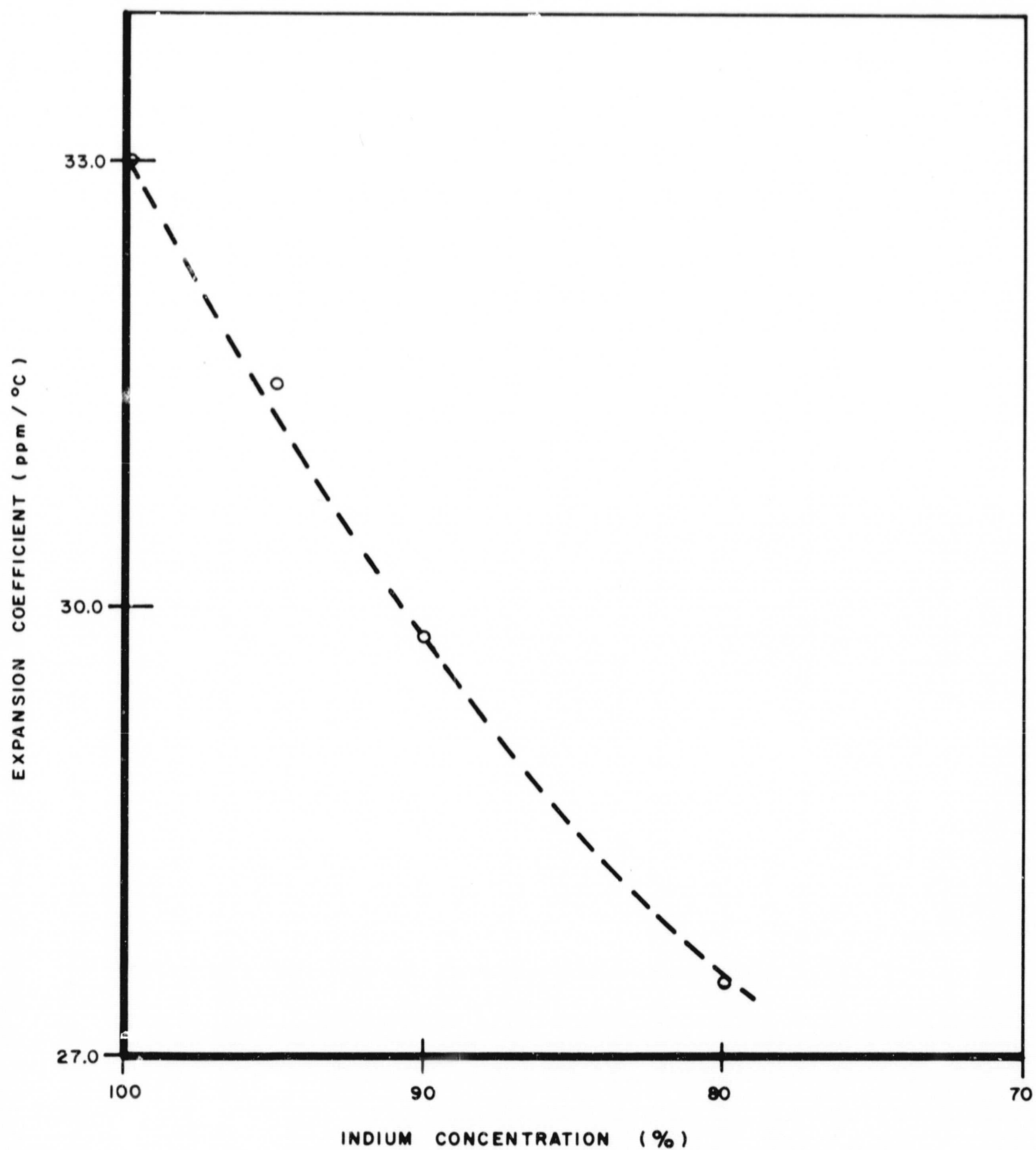


Figure 30. Expansivity in Ag-In ($20^{\circ} \leq T \leq 130^{\circ}\text{C}$)

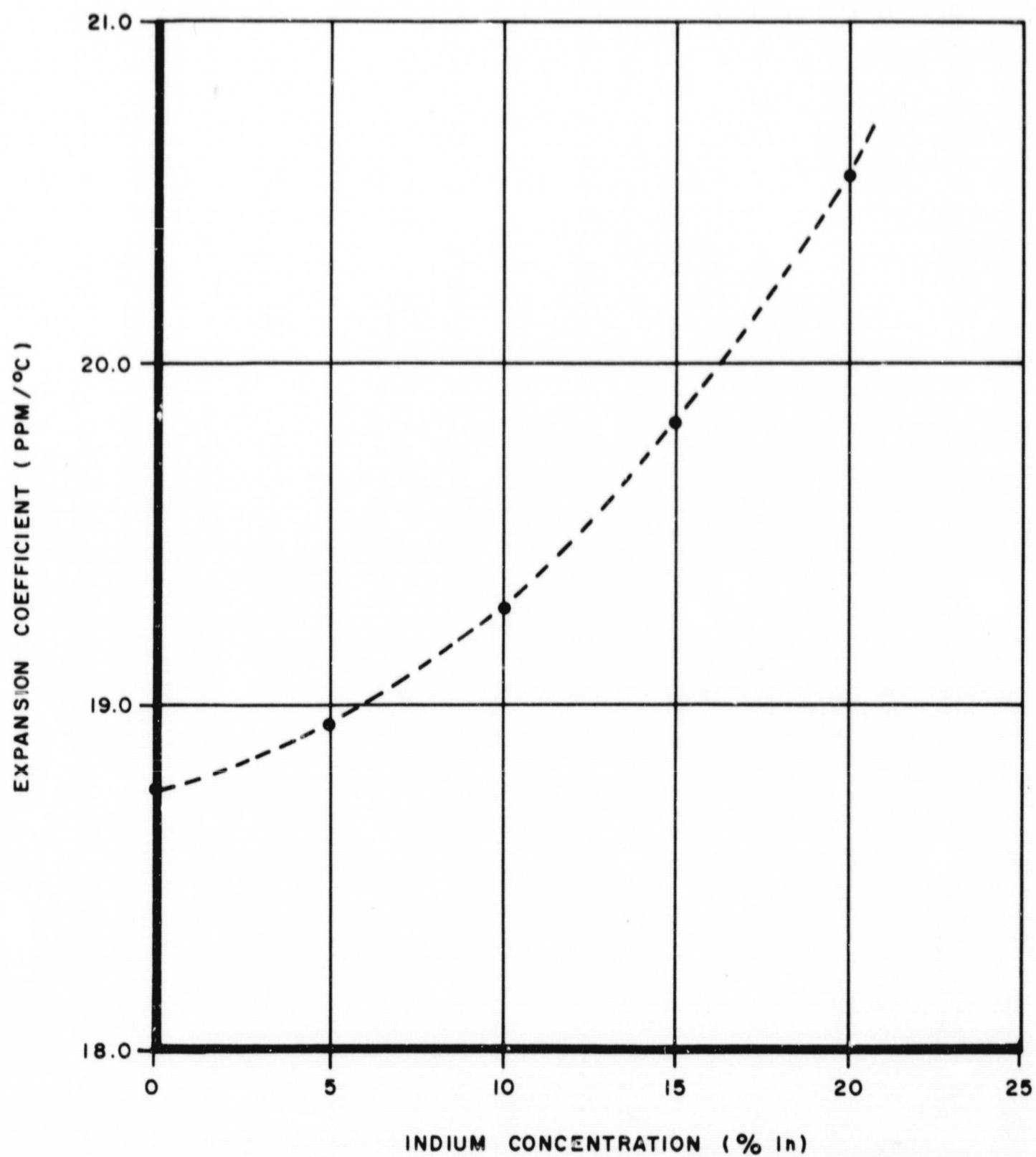


Figure 31. Expansivity In Ag-In ($20^{\circ} \leq T \leq 150^{\circ}\text{C}$)

Initially samples were cast in an induction heater, which melts and stirs the mixture simultaneously. An argon atmosphere and graphite mold were used.

Appropriate quantities of silver and indium shot were placed in the mold and melted. After a time sufficient to insure a uniform alloy, the entire system was allowed to cool and the cast rods were removed. The samples were then machined into right cylinders for measurement. It was found that this method of casting left large voids in the samples and the data generated could not be relied upon.

An alternate approach for void-free sample preparation was then attempted.

In the "art" of crystal growing, one common method of removing both voids and impurities is "gradient cooling." This is a modification of zone refining in which the entire sample is made molten, and as cooling proceeds from one end, a liquid-solid interface progresses across the sample, leveling the solute content and sweeping gas pockets and voids to one end of the sample. The apparatus commonly used for the process is a Bridgman Furnace. This is simply a wire-wound furnace with a step gradient in it. Since these are not readily available one was constructed along with an accompanying S.C.R. control unit. A typical low temperature profile is shown in Figure 32. Similar profiles exist for peak temperatures up to 1080°C.

Specimen preparation was done for both high and low temperature mixtures in the same manner. Alloys which had been mixed in the induction heater were vacuum sealed in graphite coated quartz tubes and lowered through the furnace. The peak temperature was held at 100°C above the melting point and the lowering rate was

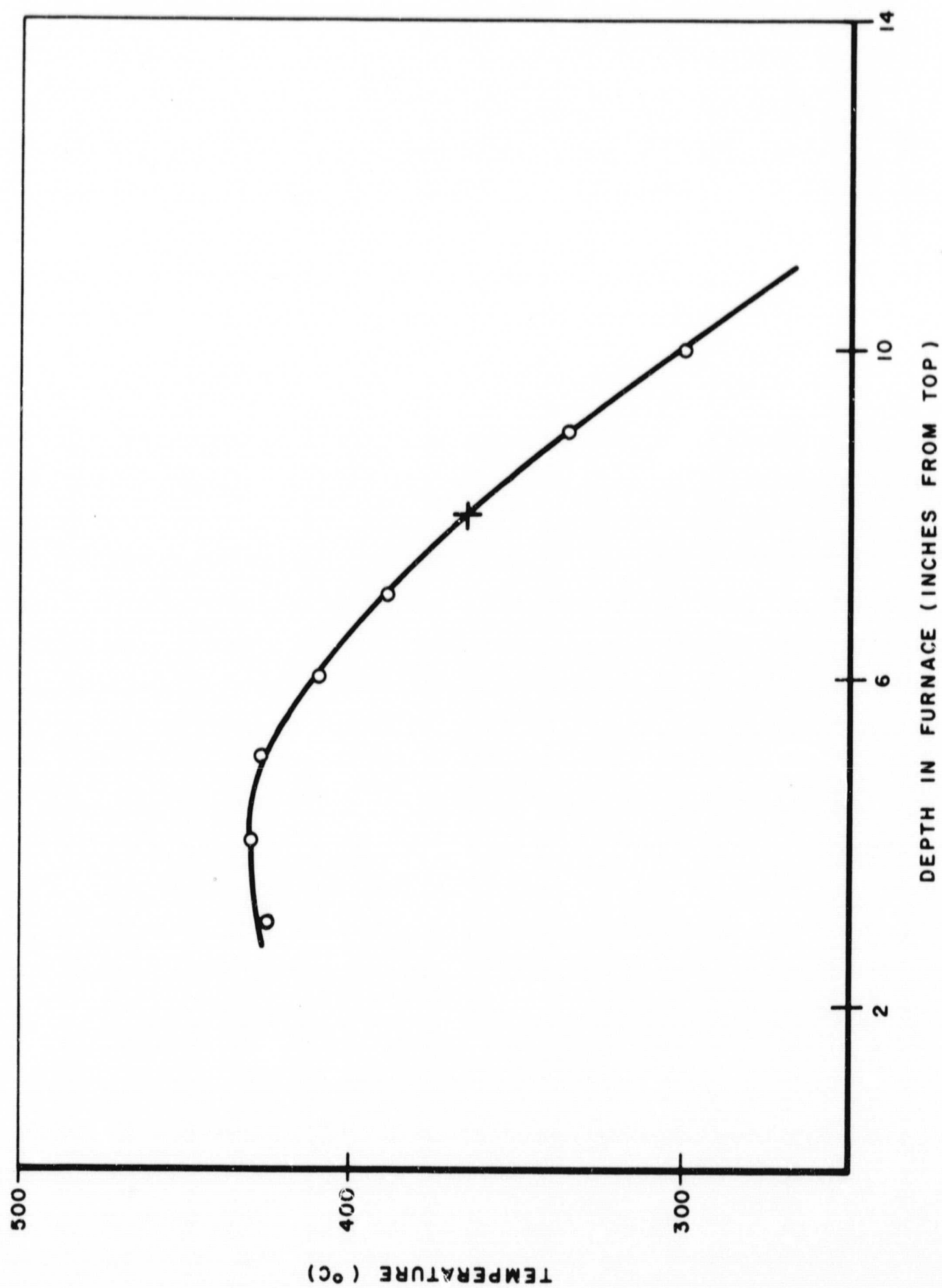


Figure 32. Bridgman Furnace Profile

7629-10-8

approximately 1 in/hr. After the samples passed completely through the furnace and had cooled, the tubes were broken and specimens slid out. The resultant slugs were void free and uniform. Slight machining was necessary to produce the right cylinders.

Results of the measurements are shown in Figure 33. Only the data for concentrations of silver greater than 50 percent are included, because difficulty in specimen preparation causes highly unreliable results from the indium rich solutions. These results indicate, as one would expect, a sharp decrease in conductivity as one perturbs the silver lattice with the poorer conductor. This again points out the advantage of using a "solid-solution" solder for connection to a heat sink, rather than a eutectic one.

2.4.8 Elastic Modulus

The elastic modulus measurements for the Ag-In system have proceeded as planned (at least in the solid solution ranges of less than 20 percent solute).

Samples were "swaged" from cast 0.5-inch diameter slugs into 0.125-inch diameter rods suitable for pulling in an Instron tester. The swaging process insured void free uniform diameter specimens at each composition and presented an attractive alternate to casting the tensile samples. Each sample was annealed for 12 hours at just below its melting point to remove the residual stress left by the swaging process.

The Instron machine used for the tensile measurements was the Model TT Universal Testing Instrument shown in Figure 34.

The machine itself consists of one static and one screw-driven cross beam. Loads may be applied in either tension or

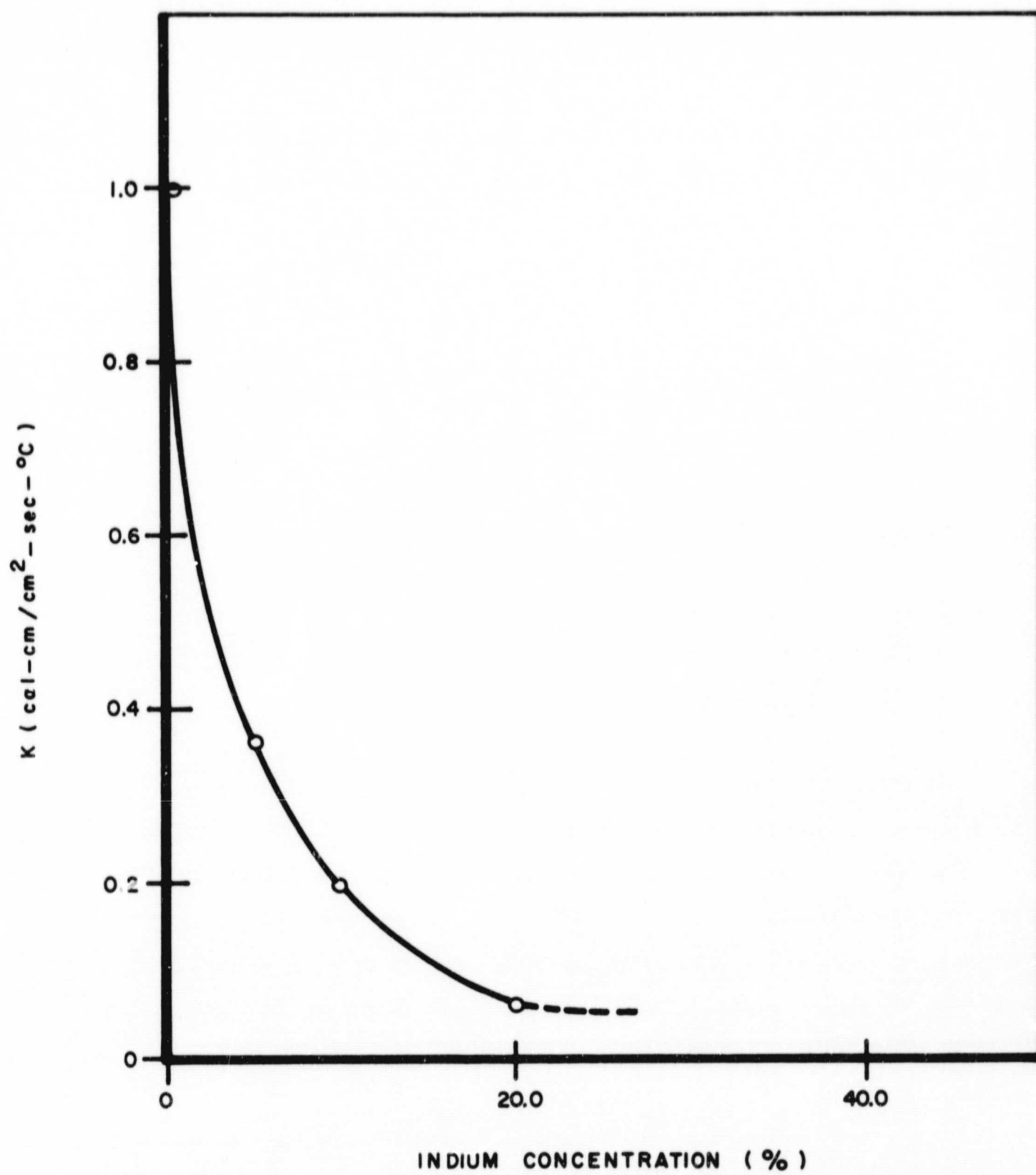


Figure 33. Thermal Conductivity of Ag-In
($T = 100^\circ\text{C}$)

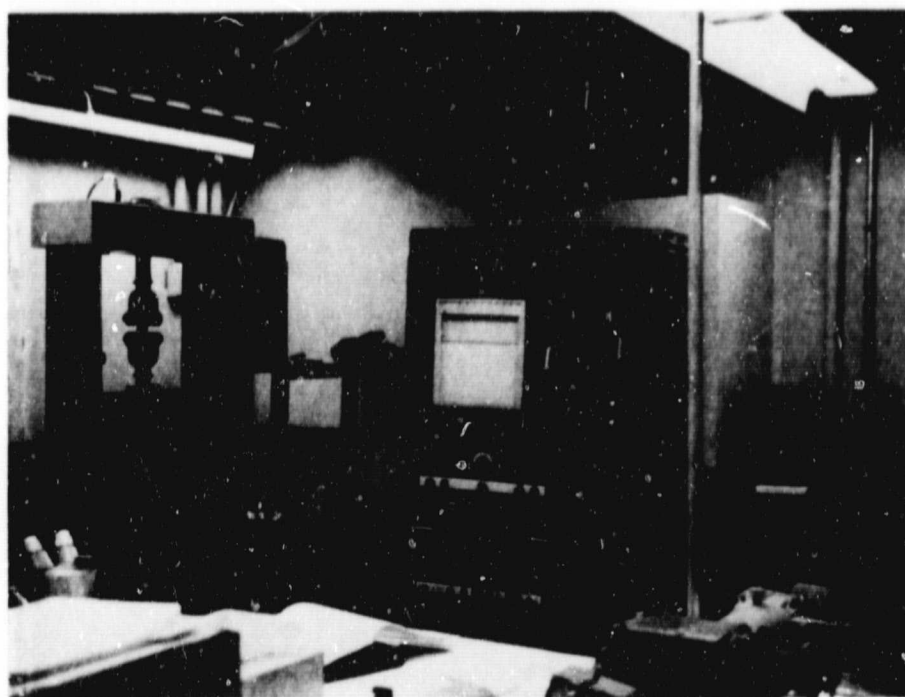


Figure 34. View of Model TT Instron Tester

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compression at any of a number of strain rates. The elongation and loading of the sample were plotted by a strip chart recorder which was an integral part of the machine. A load cell electrically drives the pen along the horizontal axis. The pen's vertical displacement is governed by a constant speed drive or, when a strain gage extensometer is used, is made proportional to the rates of elongation to gage length.

The strain gage extensometer is composed of two knife edges joined by rigid metal arms. When attached to the specimen, displacement of the knife edges beyond their natural two-inch spacing results in a measurable strain on the joint. This strain is transduced by a common resistance type strain gage into an electrical signal which is amplified and used to drive the vertical displacement of the strip recorder. Relative elongation of the specimen is plotted against the load producing the elongation. The result is a stress versus strain plot from which Youngs' modulus may be easily calculated. The only condition is that Hooke's Law be valid. This is true as long as the elastic limit of the material has not been exceeded.

The use of the strain gage extensometer greatly improves the accuracy of the measurements. This is because the primary source of error is the grosser mechanical features of the machine. There is elastic deformation of the pins and linkage holding the sample during loading which causes errors in the strain. Also, slippage of the sample between the jaws caused errors in both the strain and gage length. However, when the extensometer is used there are no deformation errors introduced because the extensometer is never subjected to loading. Equally important is the high accuracy with which the same gage length is established when the extensometer is properly used. Again, as there is no loading, there is no chance of slippage changing the gage length.

Experimental problems caused by the dependence of Young's modulus on the strain rate were avoided by testing all samples at a rate of 0.02 inches per minute. At this low strain rate the dependence is not important.

Results of the tensile tests for elastic modulus are shown in Figure 35. As one expects, the presence of indium tends to "soften" the alloy. Both curves show increases as the intermetallic regions are approached; this is another indication of the "hardness" of these materials.

It is noteworthy that data does not exist for the intermetallic regions. This is due in a large part to our inability (because of the extreme brittleness) to have compounds with near 50-50 composition machined. Figure 36 shows the results of an attempt to swage 50-50 Ag-In. At the first pass, the end of the sample is shattered into bits making further machining impossible. This is the typical behavior of intermetallic compounds and points out further why such materials are to be avoided.

2.4.9 Maximum Tensile Strength

Samples used for the elastic modulus' measurements were also used to find the tensile strength of the alloys. In this case, the specimens are pulled beyond the elastic region of the stress-strain curve, and the maximum force per unit area which the sample will take is measured. Results are shown in Figure 37 and indicate an increase in this parameter as the doping level of both lattices increases.

2.5 COMPUTER STRESS ANALYSIS

It is desirable to calculate the stress which is generated between joined members due to the disparity between their thermal

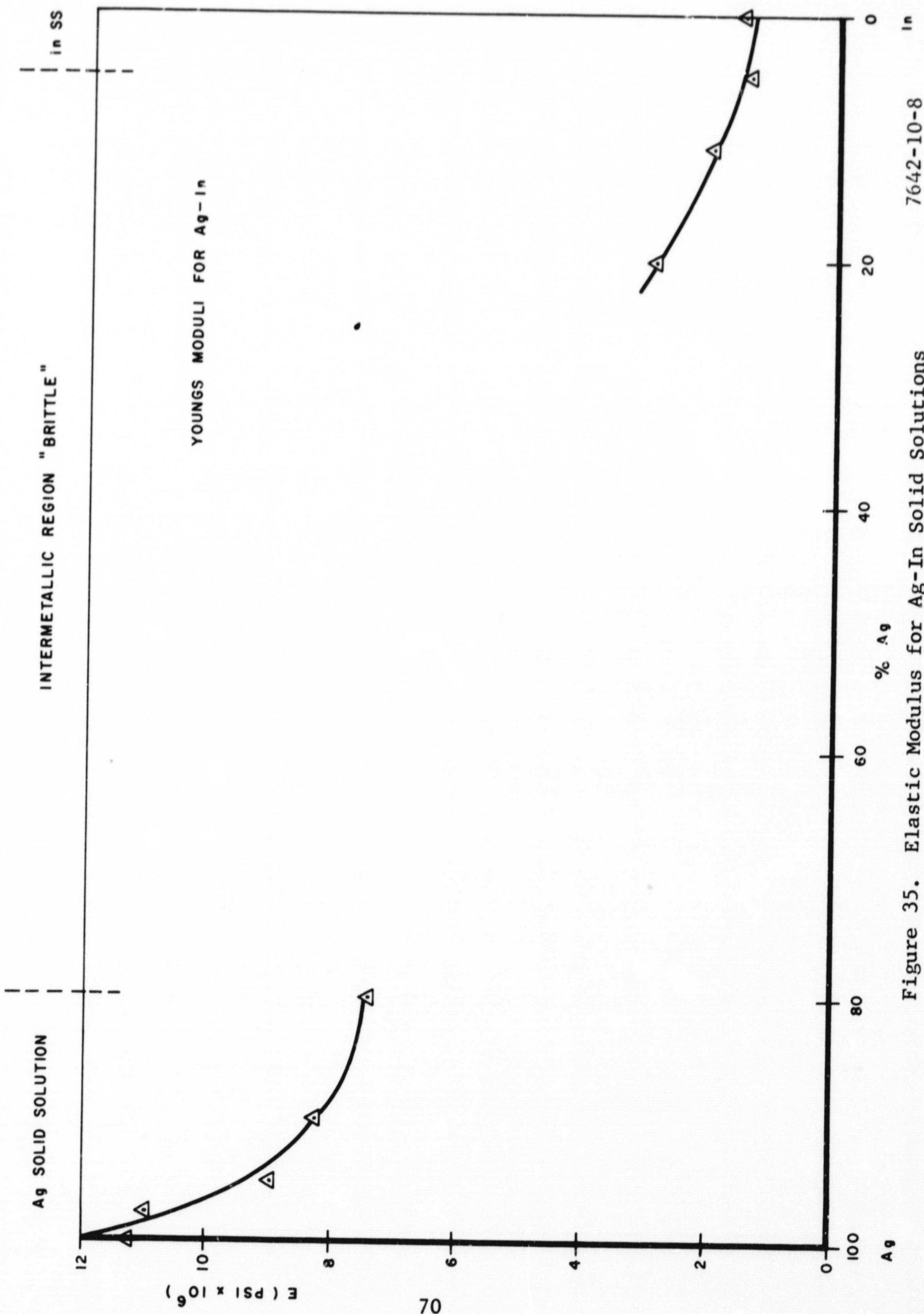


Figure 35. Elastic Modulus for Ag-In Solid Solutions

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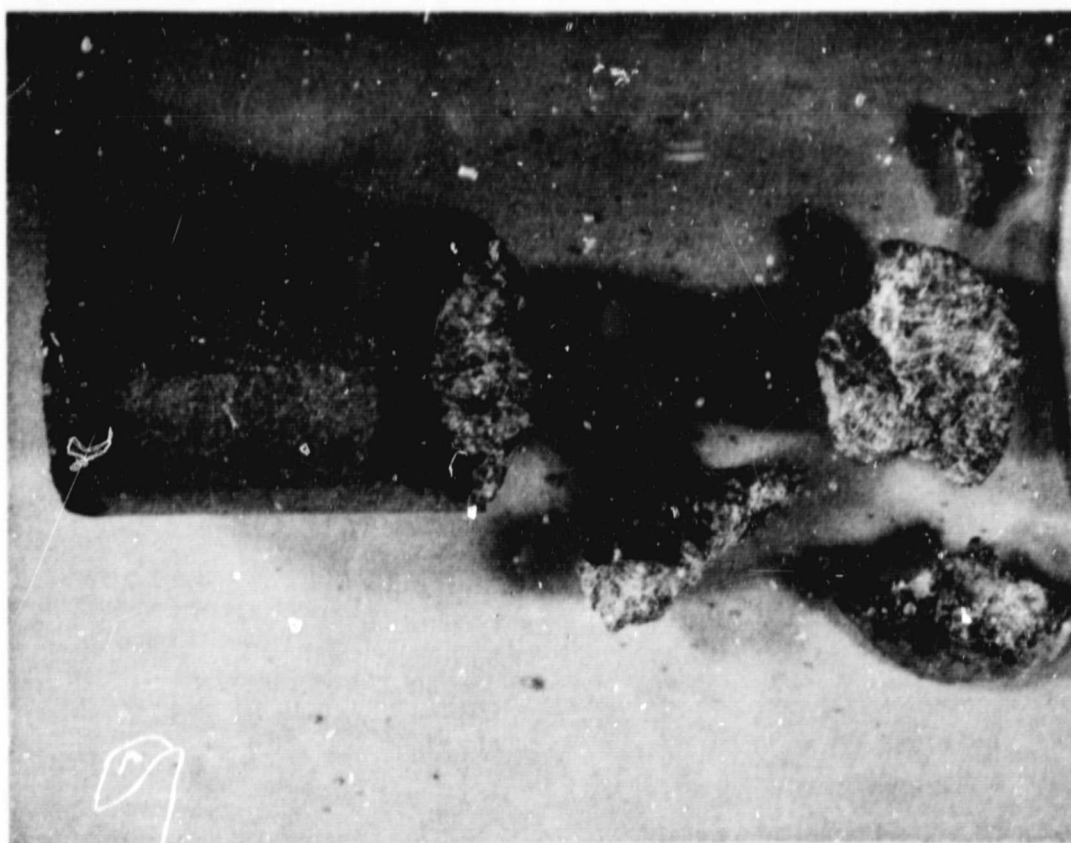


Figure 36. Results of an Attempt to Swage 50-50 Ag-In
Showing the Brittle Nature of the Material

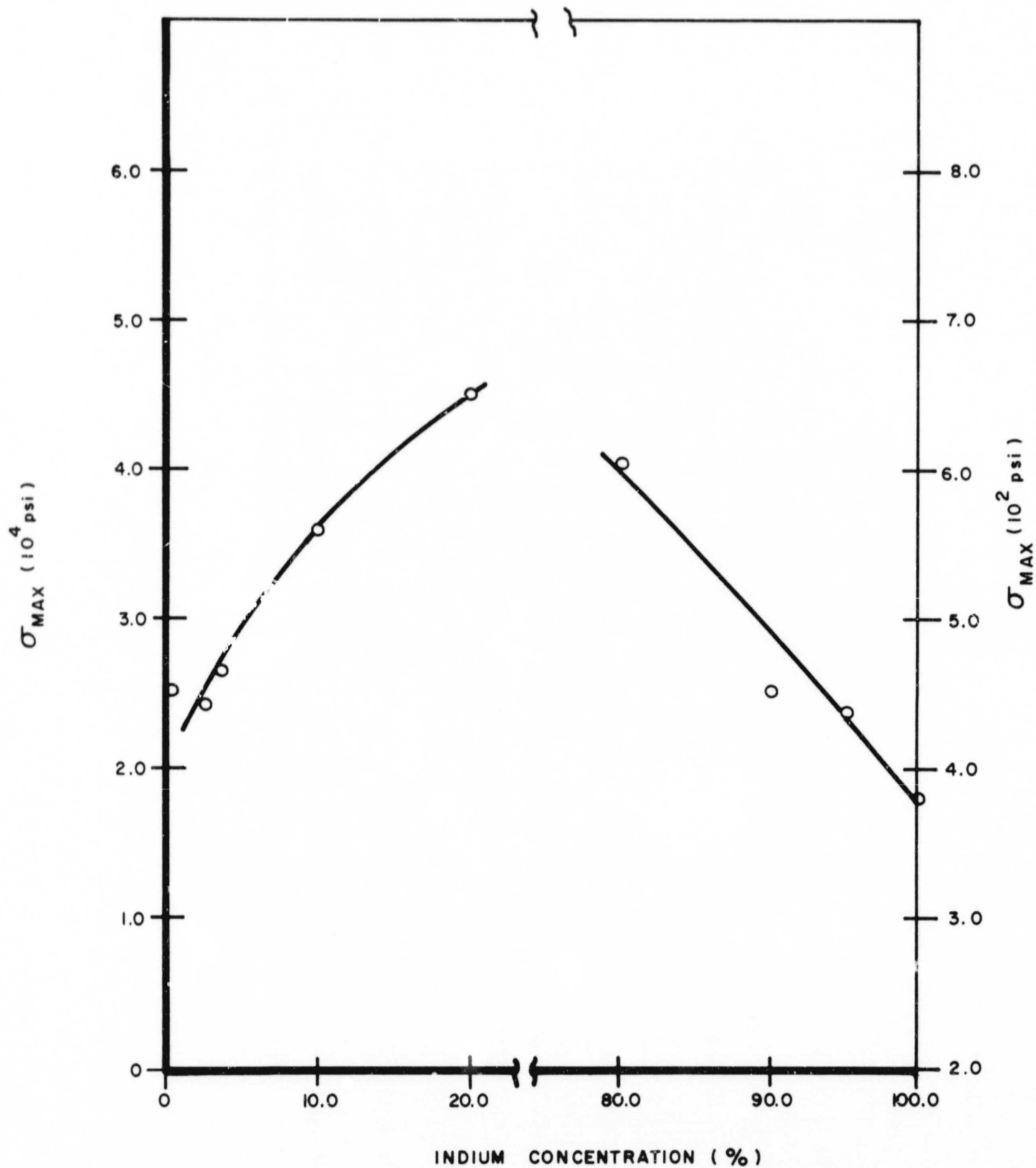


Figure 37. Tensile Strength for Ag-In

7804-1-9

expansion coefficients. From this knowledge, the required mechanical properties of solders and the desired solder thickness can be determined, which will result in a mechanically sound system since this is essentially the sole source of mechanical stress applied to the bond. A knowledge of the stress patterns in the wafer layer of a bonded system is essential for the design of sensitive junction devices, whose performance is dependent on the stress conditions at the p-n junction.

In this phase of the program, the stresses in such joined bodies have been estimated. Particular emphasis has been placed on the tri-layer system silicon-gold-molybdenum, since this is the system used for most of the experiments with large area bonds.

2.5.1 The Numerical Method

The first approach used in the determination of stress due to the bonding of dissimilar metals was a numerical one, using the equilibrium equations for the system.

These equations are derived from the force balance necessary to equilibrate a system:

In cylindrical coordinates (r, θ, z) these can be shown to be:

$$\frac{2(1-\nu)}{(1-2\nu)} \left[\frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} - \frac{u}{r^2} \right] + \frac{1}{(1-2\nu)} \frac{\partial^2 w}{\partial r \partial z} + \frac{\partial^2 u}{\partial z^2} = 0 \quad (2.5-1)$$

$$\frac{2(1-\nu)}{(1-2\nu)} \frac{\partial^2 w}{\partial z^2} + \frac{1}{(1-2\nu)} \left[\frac{1}{r} \frac{\partial u}{\partial z} + \frac{\partial^2 u}{\partial r \partial z} \right] + \frac{1}{r} \frac{\partial w}{\partial r} + \frac{\partial^2 w}{\partial r^2} = 0 \quad (2.5-2)$$

where u and w are the displacements in the r and z directions.
 ν is the Poisson Ratio, and axial symmetry is assumed. In terms of these displacements the principal stresses are given by:

$$\sigma_r = \frac{E}{(1+\nu)(1-2\nu)} \left[(1-\nu) \frac{\partial u}{\partial r} + \nu \left(\frac{u}{r} + \frac{\partial w}{\partial z} \right) \right] - \frac{EkT}{(1-2\nu)} \quad (2.5-3)$$

$$\sigma_\theta = \frac{E}{(1+\nu)(1-2\nu)} \left[(1-\nu) \frac{u}{r} + \nu \left(\frac{\partial u}{\partial r} + \frac{\partial w}{\partial z} \right) \right] - \frac{EkT}{(1-2\nu)} \quad (2.5-4)$$

$$\sigma_z = \frac{E}{(1+\nu)(1-2\nu)} \left[(1-\nu) \frac{\partial w}{\partial z} + \nu \left(\frac{u}{r} + \frac{\partial u}{\partial r} \right) \right] - \frac{EkT}{(1-2\nu)} \quad (2.5-5)$$

$$\tau_{rz} = \frac{E}{2(1+\nu)} \left(\frac{\partial w}{\partial r} + \frac{\partial u}{\partial z} \right) \quad (2.5-6)$$

$$\tau_{r\theta} = \tau_{z\theta} = 0 \quad (2.5-7)$$

Hence in order to calculate the principal stresses, one must solve the differential equations (2.5-1) and 2.5-2) for the displacements and use equations (2.5-3) through (2.5-7) to obtain the stresses.

One way to solve such second order equations is through numerical difference methods. In this approach one divides up the problem area with a grid and makes a point-by-point solution using linear approximations along with their boundary conditions which were reduced to numerical approximations. For the homogeneous second derivative terms (e.g., $\frac{\partial^2 u}{\partial r^2}$) no trouble was encountered in the reduction. However, the cross-second derivatives (e.g., $\frac{\partial^2 u}{\partial r \partial z}$) could not be approximated by this method at the boundaries and

interfaces. By using so-called "backward" or "forward" difference approaches this was overcome and solutions were obtained. In spite of this, the values for the shear stresses in either case were radically different, depending upon which approximation was employed. Furthermore, the solutions converged very slowly.

In view of these problems, the numerical approach was abandoned, and an attempt at an analytical solution was initiated.

2.5.2 Analytical Solution by Superposition

An analytical solution⁽⁸⁾, as described in this section, was initiated to determine the resultant stresses in the axial, radial and hoop directions as well as the shear stress. The method employed is to determine these stresses under four stress conditions. The sum of the various stresses for each condition will yield the desired solution. The method, therefore, is one of superposition, in which surface tensile forces are applied to assure that in the summation, the stress at the surface of the body is zero.

2.5.3 Solution I

Two cylindrical bodies, as depicted in Figure 38(a), of differing materials are allowed to experience a thermal excursion prior to being joined. Each cylinder is allowed to expand unconstrained according to its thermal expansion coefficient with the residual stress being equal to zero.

2.5.4 Solution II

Radial stress is then applied to the circumference of both cylindrical bodies to bring their two radii equal. The stress applied results in equal work being done on each body to bring them a common radius. This is depicted in Figure 38(b). Under this condition

$$\sigma_z = \tau_{rz} = 0$$

$$\sigma_\theta = \sigma_r = \sigma_1 \text{ for material No. 1}$$

$$\sigma_\theta = \sigma_r = \sigma_2 \text{ for material No. 2}$$

where

σ_z = is the normal strain in the z direction

σ_r = is the radial stress

σ_θ = is the hoop stress

σ_1 and σ_2 are the applied radial stress at the circumferences of the two bodies.

2.5.5 Solution III

The two bodies are joined together and are then subjected to an applied radial stress at the circumference which is equal and opposite to the stresses applied in the previous case. This condition is depicted in Figure 38(c). The solution becomes

$$\sigma_r = \frac{\partial}{\partial z} \left[\nu \nabla^2 \phi - \frac{\partial^2 \phi}{\partial r^2} \right] \quad (2.5-8)$$

$$\sigma_z = \frac{\partial}{\partial z} \left[(2-\nu) \nabla^2 \phi - \frac{\partial^2 \phi}{\partial z^2} \right] \quad (2.5-9)$$

$$\sigma_\phi = \frac{\partial}{\partial z} \left[\nu \nabla^2 \phi - \frac{1}{r} \frac{\partial \phi}{\partial r} \right] \quad (2.5-10)$$

$$\tau_{rz} = \frac{\partial}{\partial r} \left[(1-\nu) \nabla^2 \phi - \frac{\partial^2 \phi}{\partial z^2} \right] \quad (2.5-11)$$

$$\phi = \sin k z \left[a_0 J_0(ikr) + a_1(ikr) J_1(ikr) \right] \quad (2.5-12)$$

where τ_{rz} is shear stress and ν is Poisson's ratio for the materials involved. The step function σ_r at the circumference is expanded in a Fourier cosine series and the solution becomes a series consisting of the Fourier series and modified Bessel functions of the first kind.

The solution leaves small residual stresses (σ_z) at the ends of the cylinder which must be eliminated if accurate results are to be obtained.

2.5.6 Solution IV

Figure 38(d) depicts the residual stress induced by Solution III. This must be corrected to obtain more precise results. A solution that satisfies the equations of equilibrium for this case is:

$$\begin{aligned} \sigma_z &= f(z) * A_z(r) \\ \tau_{rz} &= \frac{-f'(z)}{k} * A_{rz}(r) \\ \sigma_r &= \frac{-f''(z)}{k^2} * A_r(r) \\ \sigma_\phi &= \frac{-f''(z)}{k^2} * A_\phi(r) \end{aligned} \quad (2.5-13)$$

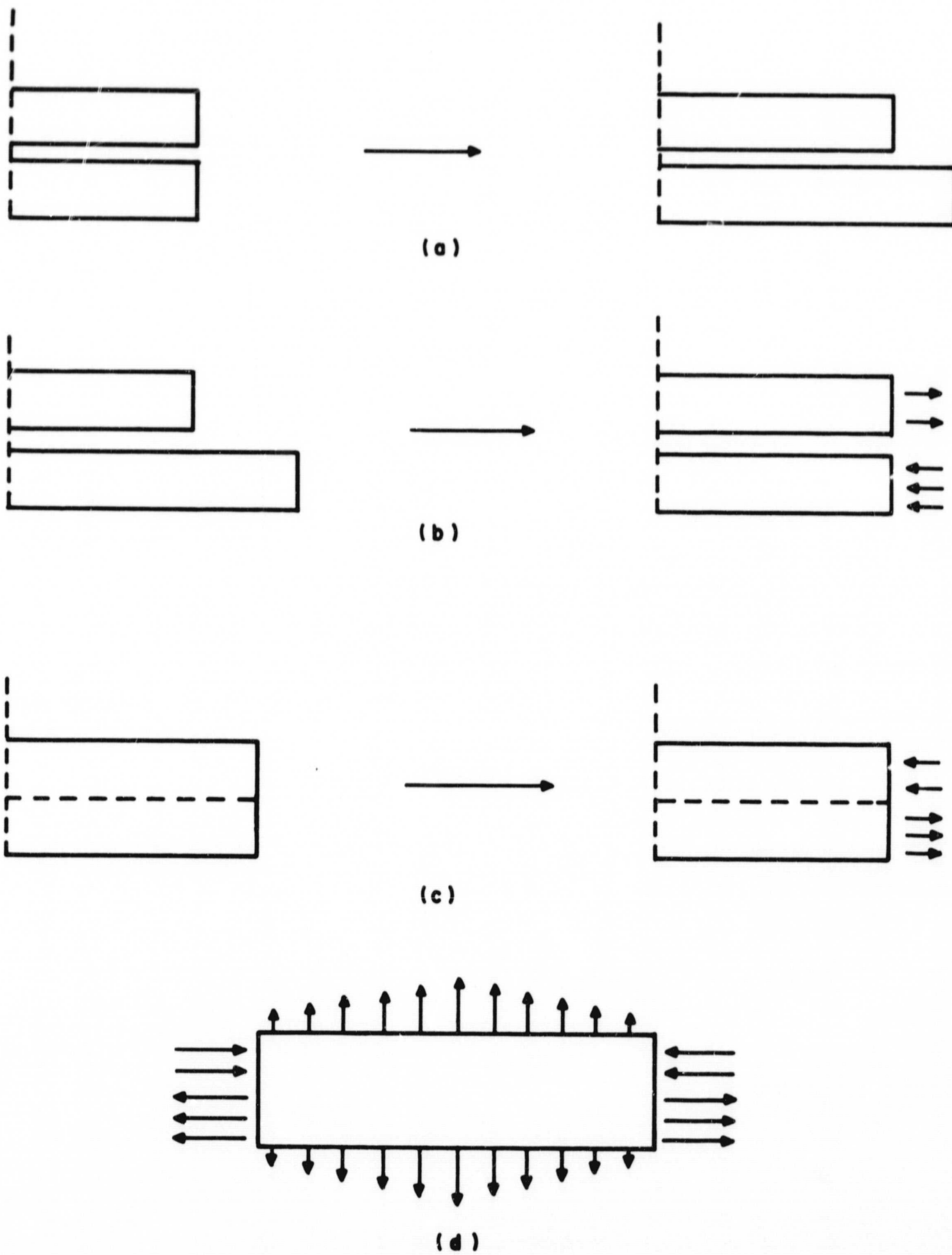


Figure 38. 4-Step Stress Calculation

where the A's are the portions of Solutions III that are functions of r. The boundary conditions on $f'(z)$ are

$$f'(z) = 0 \text{ at } z = 0, 1$$

$$f'(z) = \text{maximum at the material interface.}$$

2.5.7 Final Solution

The final stresses are obtained by adding the stresses in each solution.

For example:

$$\tau_{rz} = \tau_{rz_I} + \tau_{rz_{II}} + \tau_{rz_{III}} + \tau_{rz_{IV}} \quad (2.5-14)$$

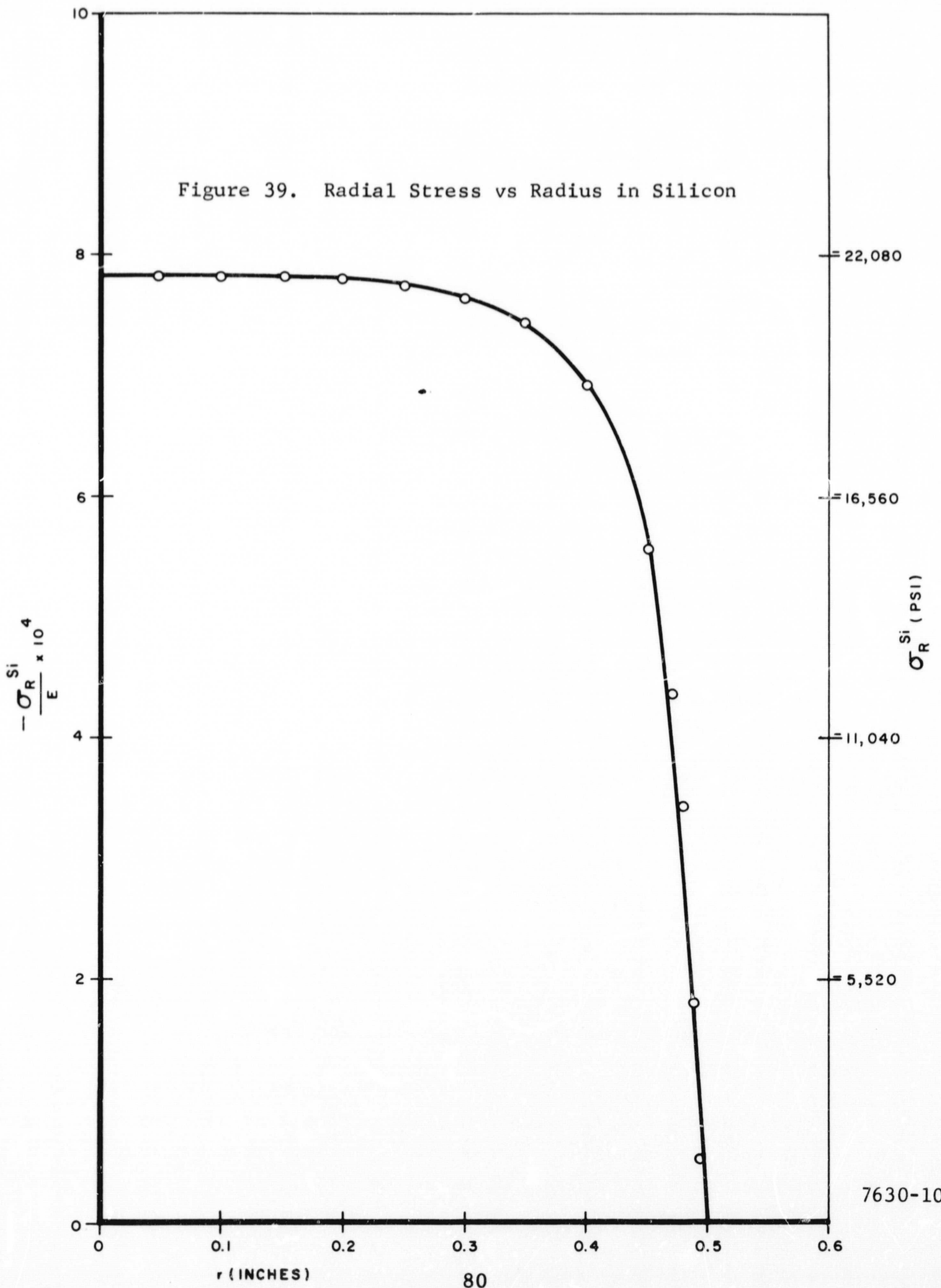
A similar procedure is employed to determine all of the remaining stresses.

These four solutions and their summation were computed by programming Motorola's GE 415 system. A copy of the computer program is given in Section 2.5.9.

2.5.8 Results

Calculations were performed for a 1-inch silicon wafer bonded with gold solder to a molybdenum heat sink. The respective thicknesses were 20, 2, and 125 mils while the expansion coefficients are 3.3, 14.3, and 5.5 in units of ppm/°C. Figures 39, 40, 41 and 42 show the radial dependences of the pertinent stresses in the silicon wafer after an excursion of -400°C; the left ordinate gives the reduced stress (σ/E), while the right ordinate shows the actual stress in psi. A positive σ represents a tension force whereas a negative one means the body is under compression.

Figure 39. Radial Stress vs Radius in Silicon



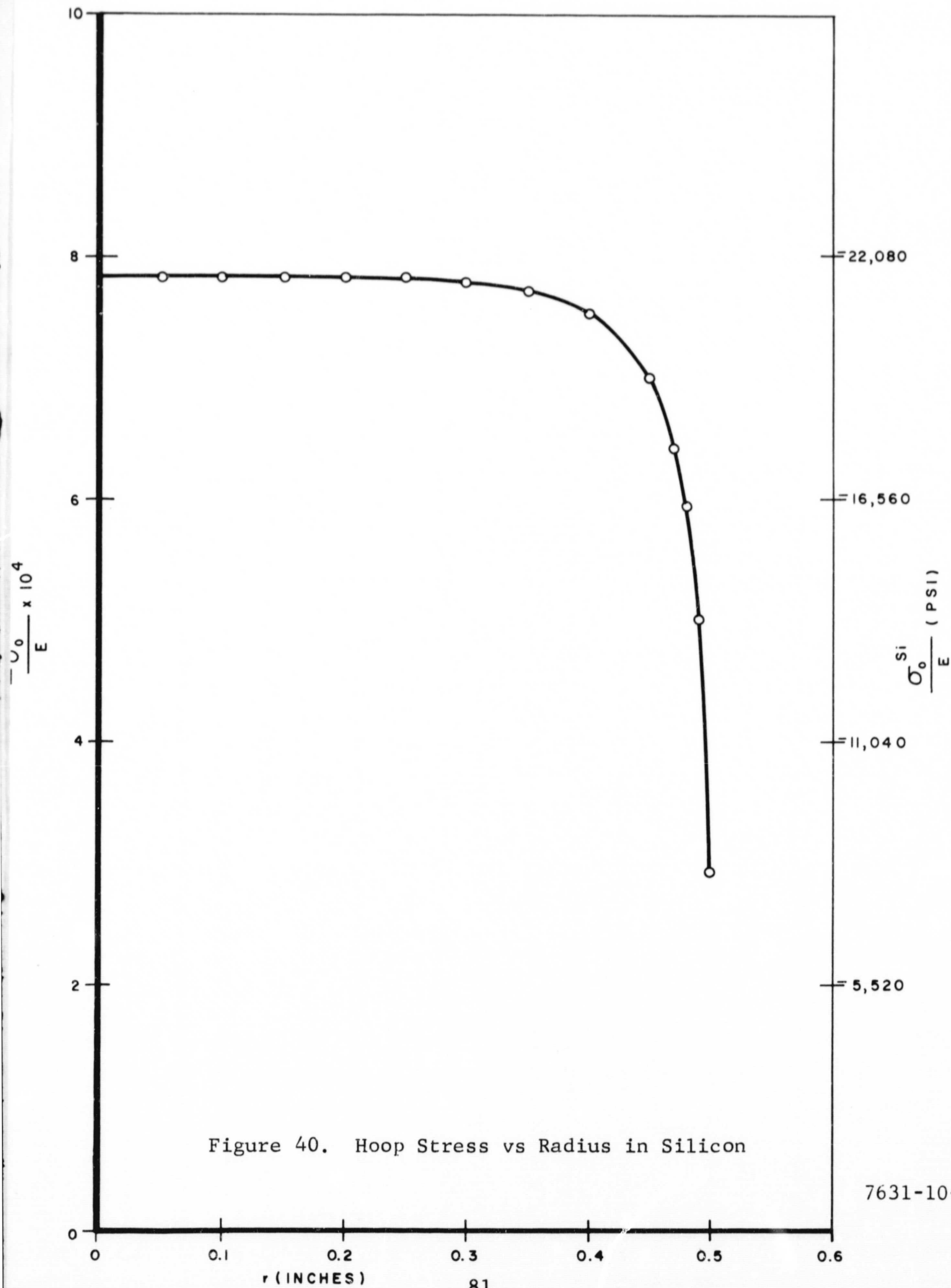


Figure 40. Hoop Stress vs Radius in Silicon

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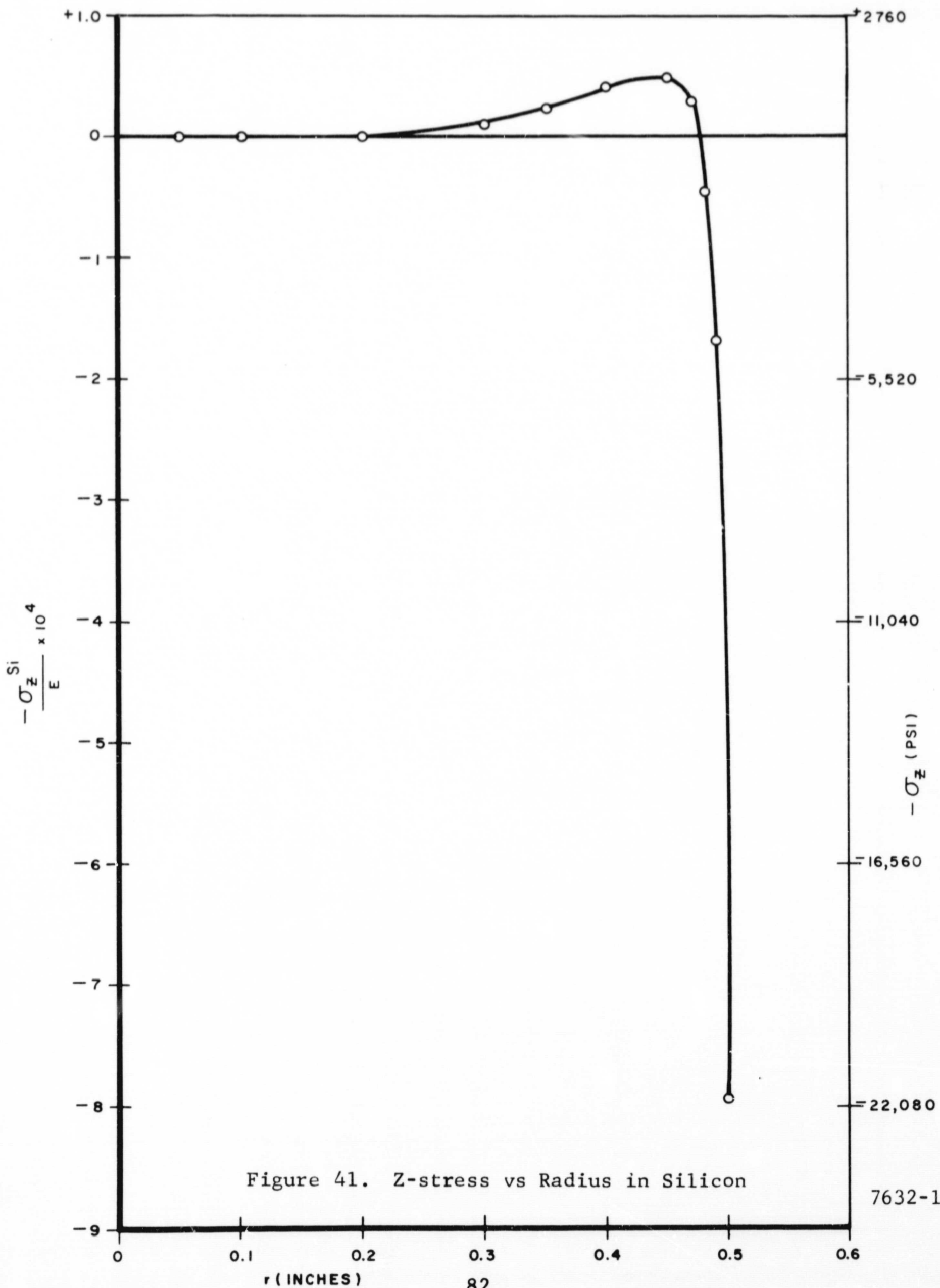
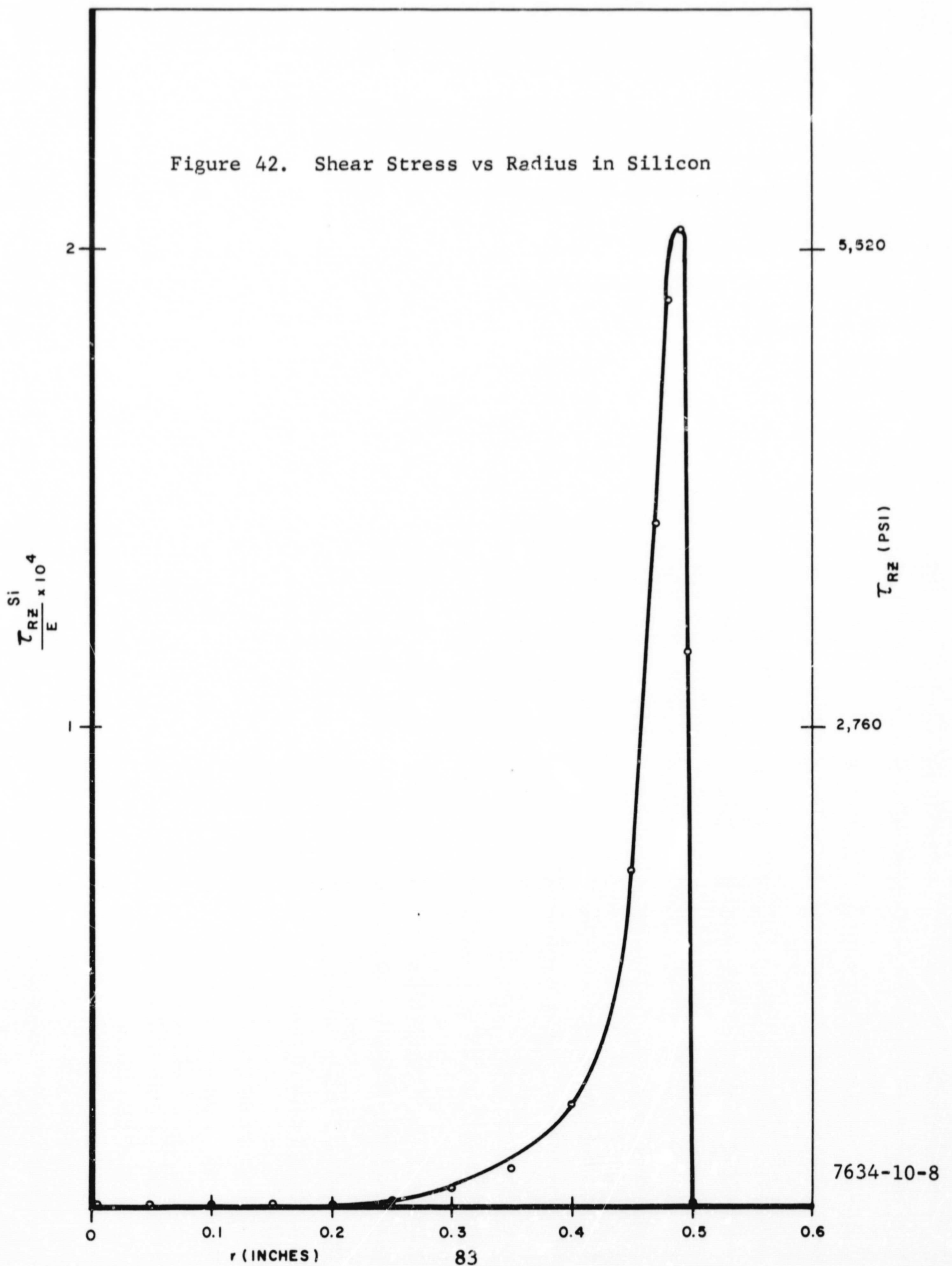


Figure 41. Z-stress vs Radius in Silicon

7632-10-

Figure 42. Shear Stress vs Radius in Silicon



7634-10-8

These results clearly show that upon cooling, a bonded silicon wafer is under considerable compressive force in the radial and "hoop" directions ($\approx 20,000$ psi), and the buckling experienced in the earlier stages of this program seems to be explained. Figure 41 shows a "Z" stress peak near the extreme of the wafer, and one might anticipate a peeling effect to follow as the wafer size increases.

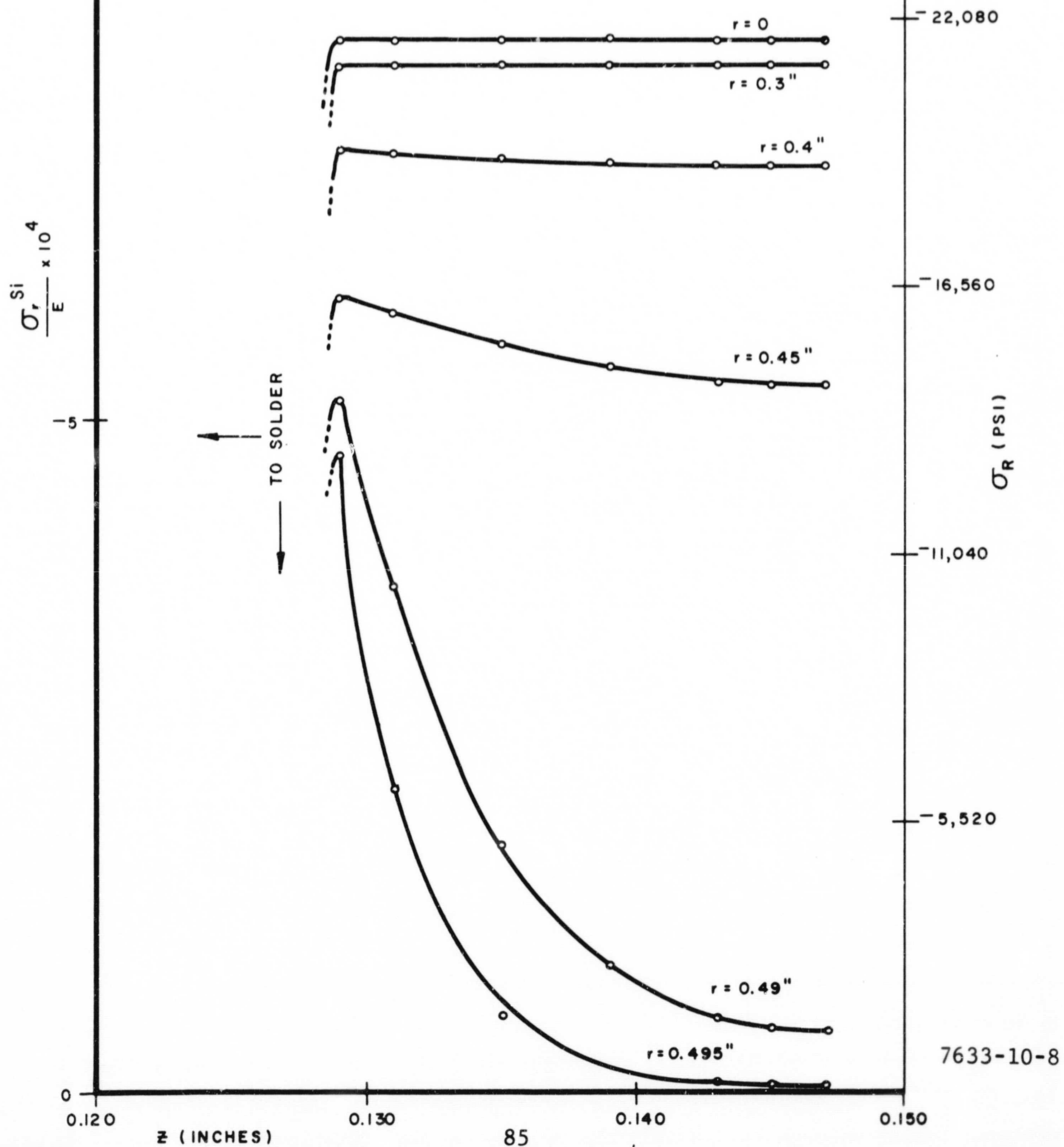
The results shown in Figure 42 demonstrate that the shear forces are considerably less than the tensile ones. This is perhaps due to the fact that the surface shear interaction actually present in the physical system is replaced in the computer calculation by an "effective tensile force," and some of the true shear shows up in the rather large tensile forces.

The "Z" dependence of the radial stress is shown in Figure 43 parameterized by the radius, and demonstrates the expected decrease in the forces as one moves away from the bonding interface and toward the wafer edge. It is noteworthy, however, that the top surface of the wafer is not stress-free as one might hope. Part of this may be due to the method of calculation of these boundary forces; however, it is felt that the presence of some non-zero stress on the surface is real, and that stress sensitive devices in this region would be affected.

The preceding figures may be condensed into a "radial-stress surface" sketched in Figure 44. Any point in the surface represents the magnitude of the stress at a given (r,z) coordinate in the silicon wafer.

The computer program yields similar data for both the molybdenum substrate and the solder layer. Curves for the pertinent data are given in Figures 45, 46, 47, and 48. These have the same

Figure 43. Radial Stress vs "Z" in Silicon



7633-10-8

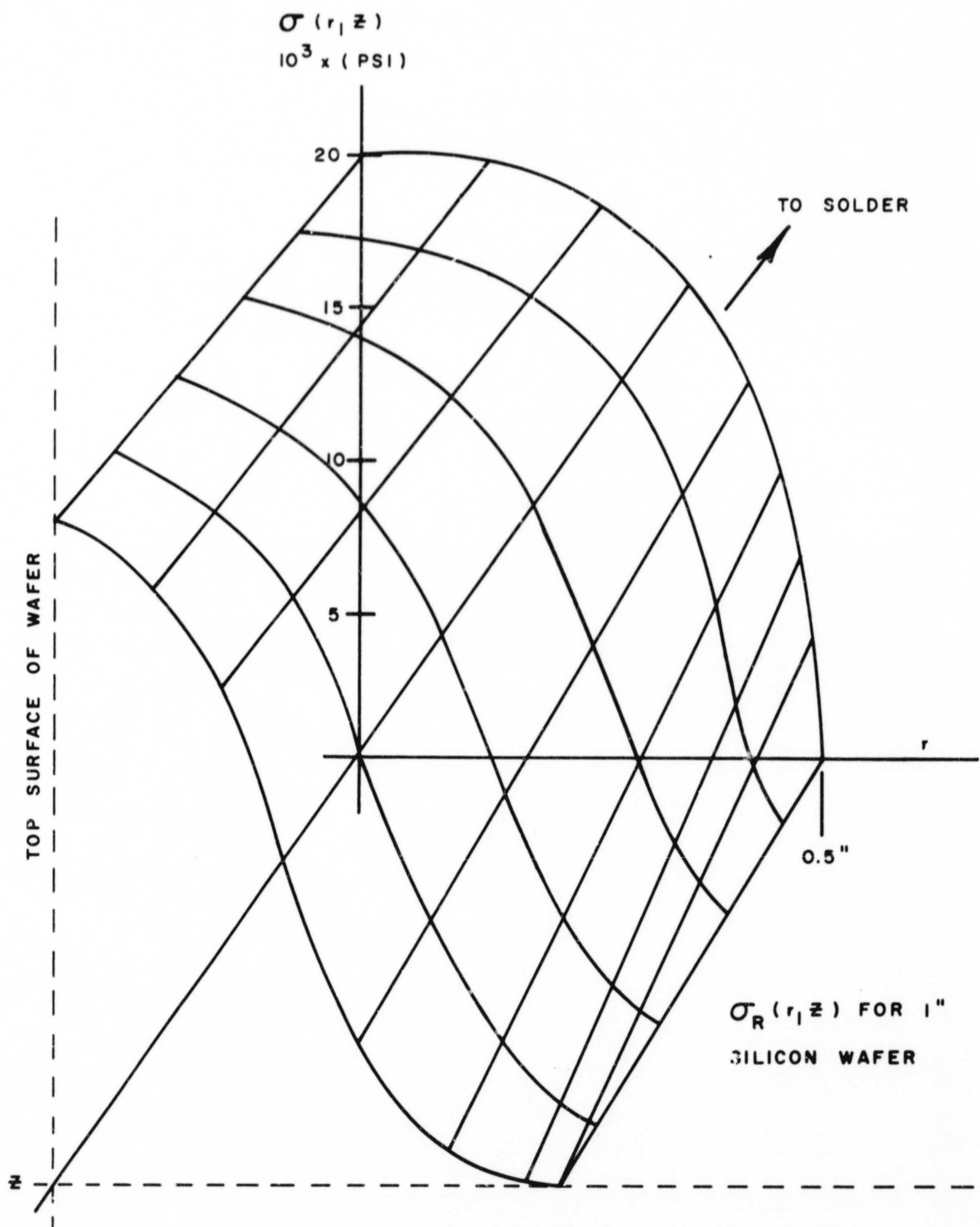


Figure 44. Radial Stress Surface for Silicon

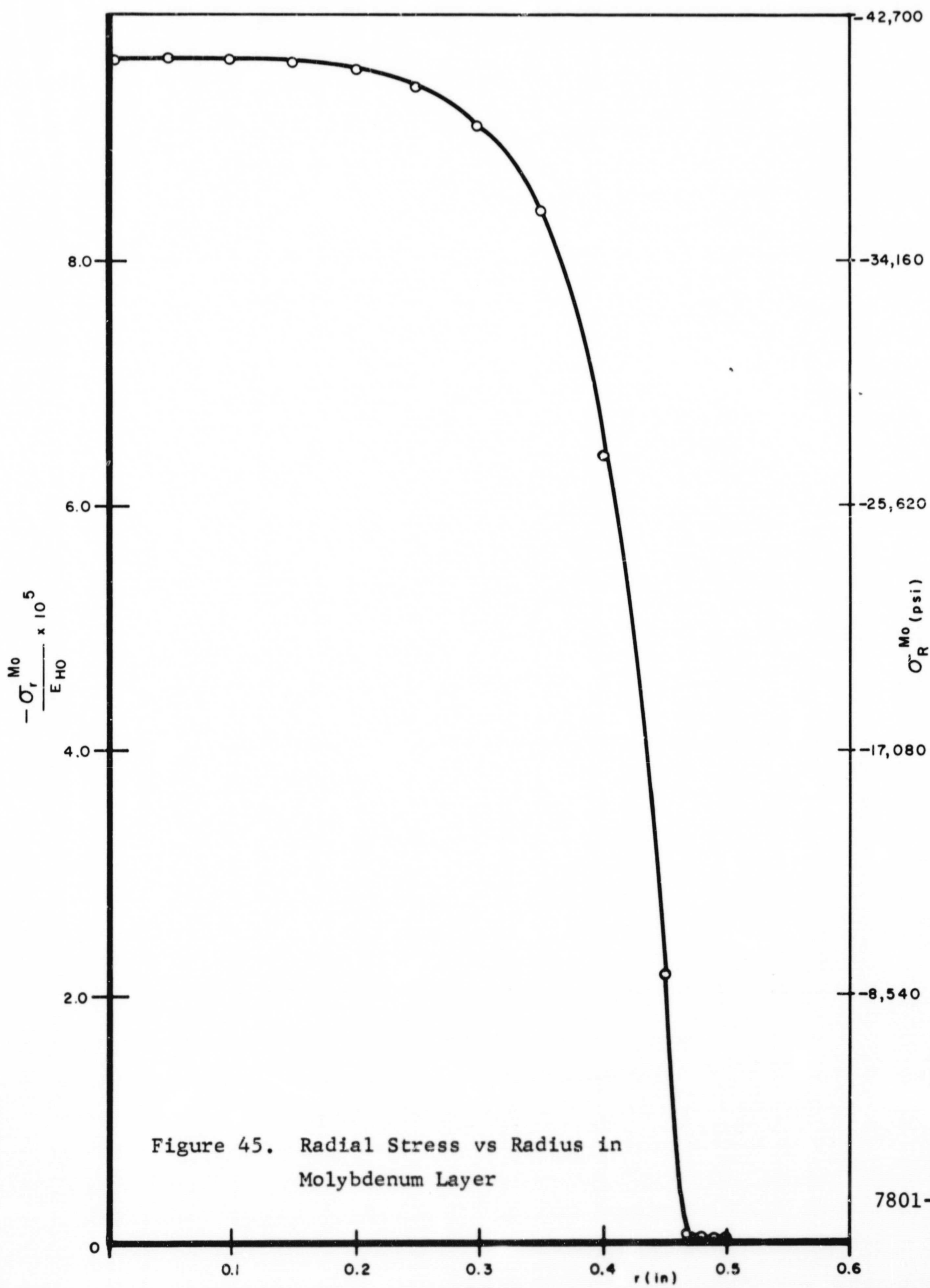


Figure 45. Radial Stress vs Radius in Molybdenum Layer

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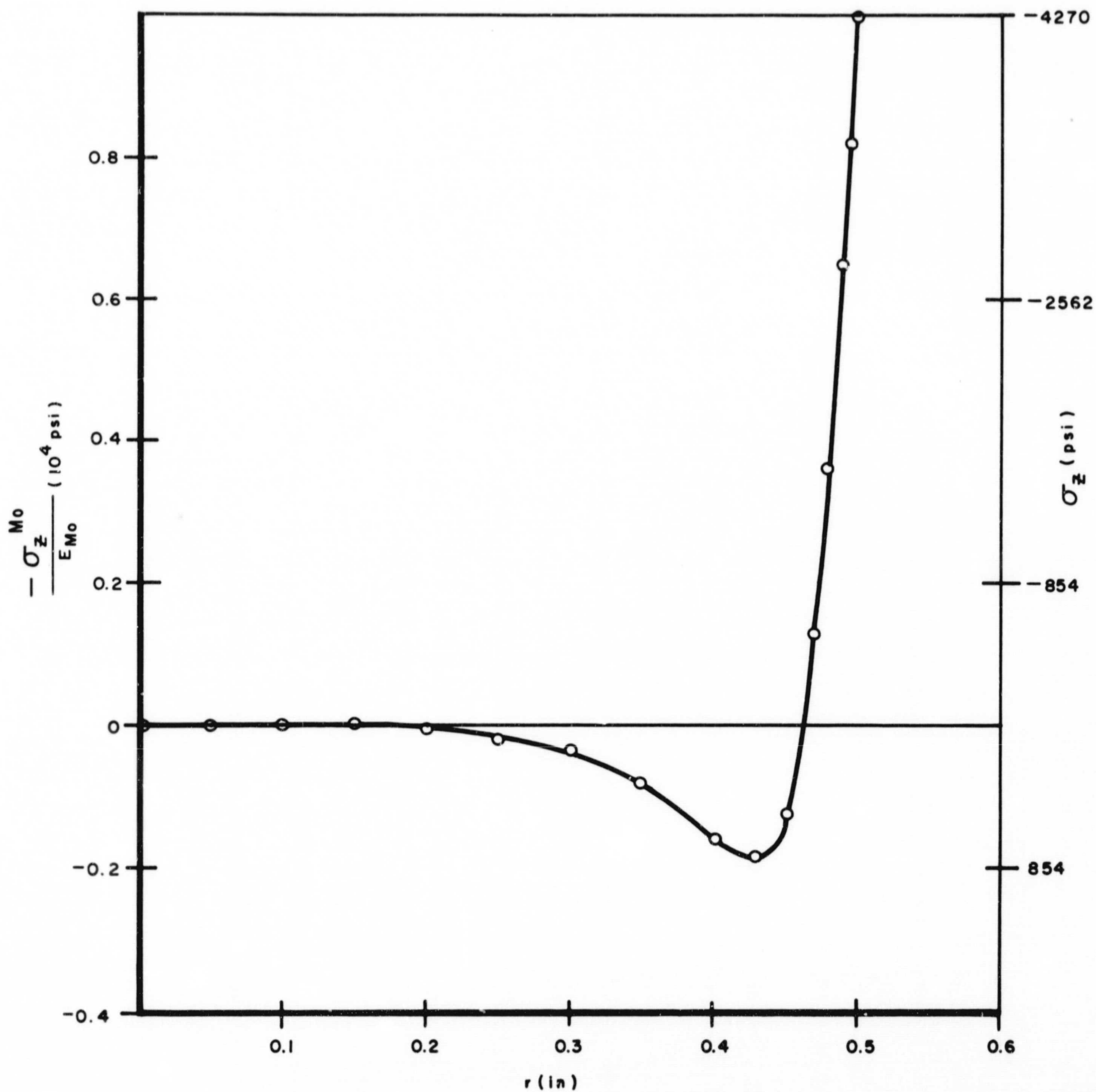
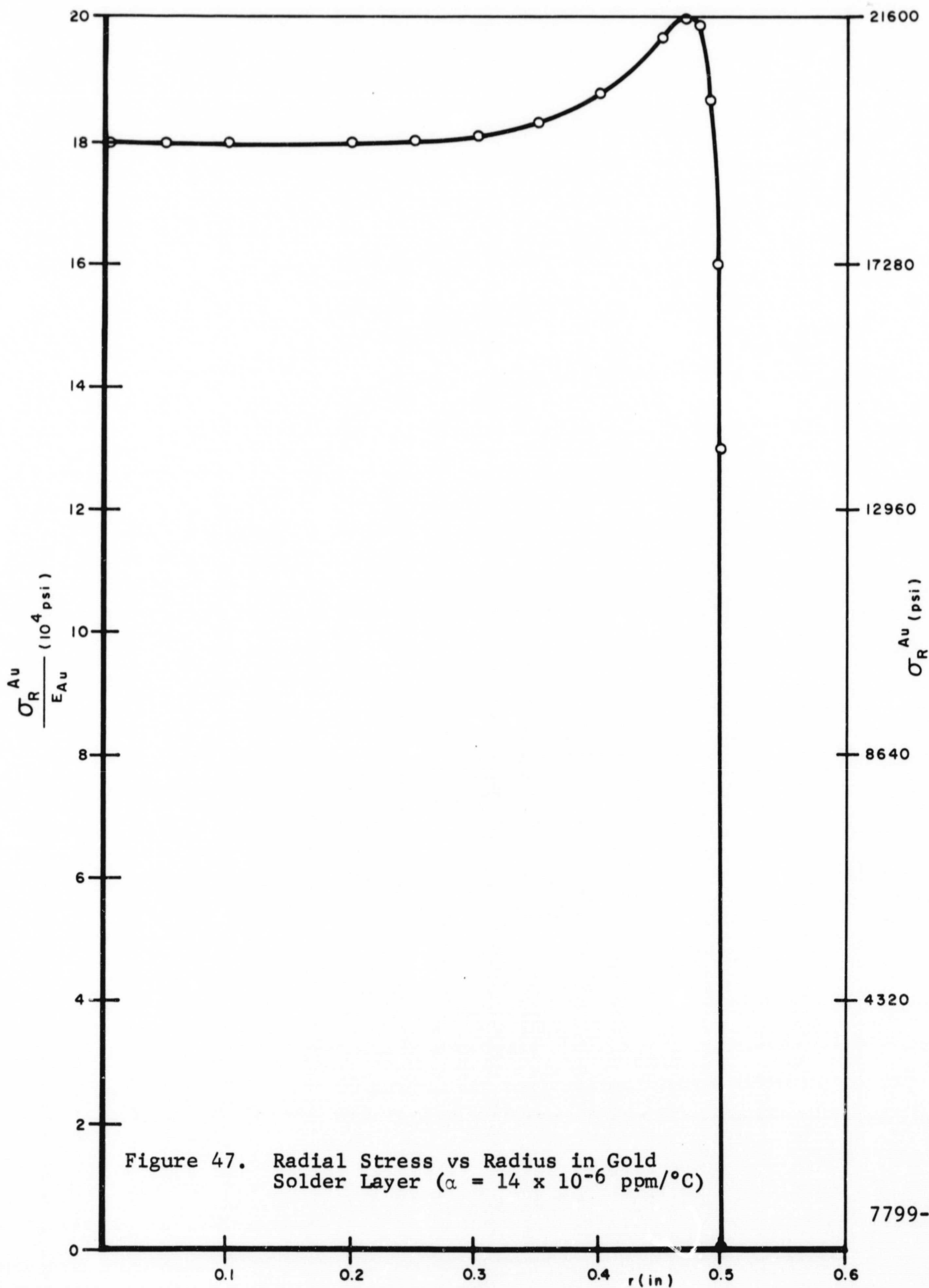


Figure 46. "Z" Stress vs Radius in Molybdenum



7799-1-9

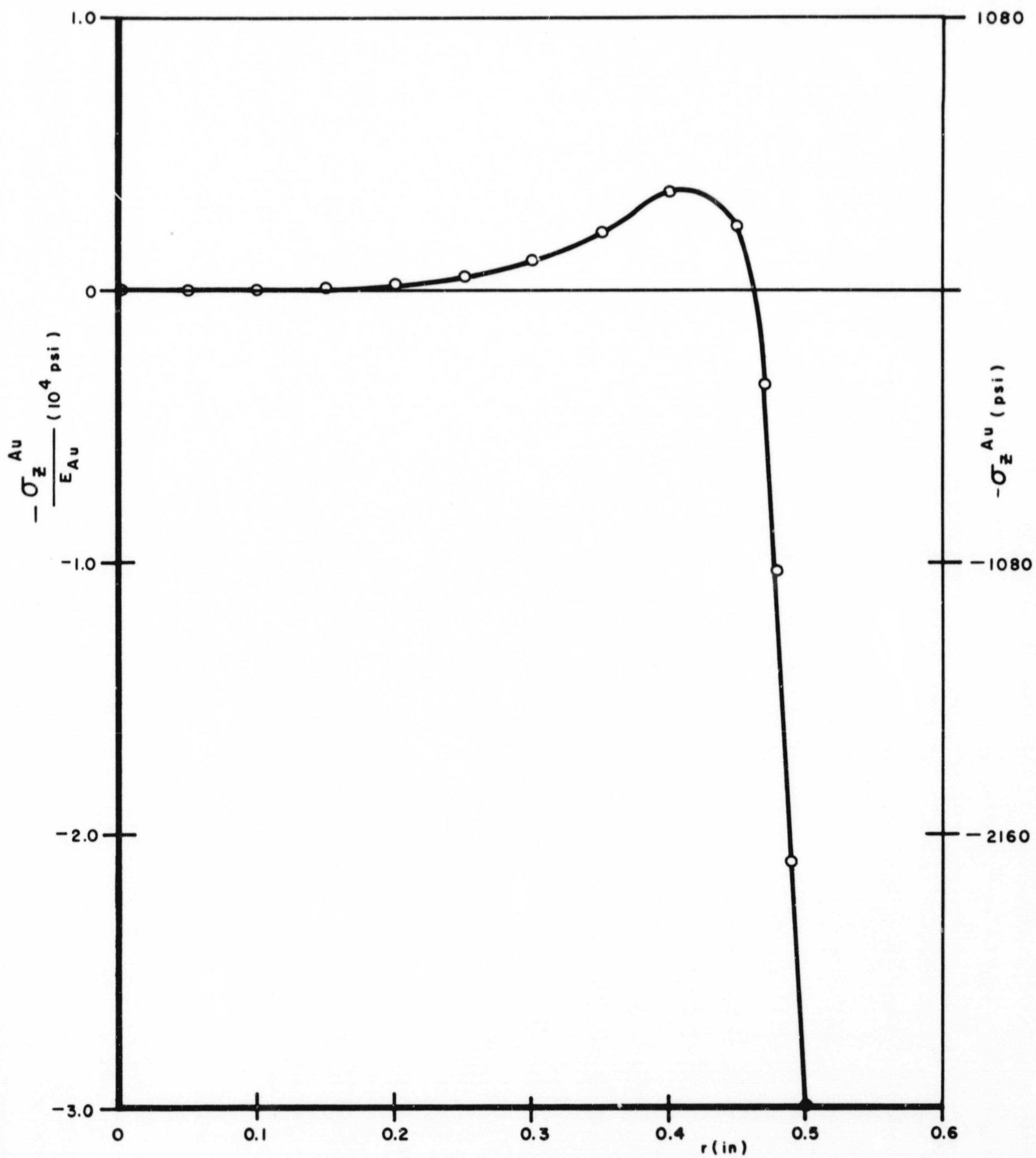


Figure 48. "Z" Stress vs Radius in Solder

7800-1-9

characteristic shape as silicon, with slightly differing magnitudes. For the solder layer the signs are reversed, since upon cooling it is in tension, having the highest expansion coefficient.

An interesting calculation has been performed to study the effects of using solder materials with different coefficients of expansion. Sample calculations have been done to determine the radial stress as a function of the expansivity of the solder. These data are summarized in Figure 49.

It should be noted that the stress levels in both the wafer and substrate appear only weakly dependent on the solder expansivity. This is probably due in part to the fact that calculations maintained the same elastic modulus for the solder (namely pure Au) while varying the expansion coefficient and also partly due to the thinness of the solder. The very thin layer would be transparent to a good part of the applied stress of the heat sink. The flat region of the solder curve is due to the fact that a plastic approximation was employed, and stresses beyond 20,000 psi exceed the elastic limit of the solder and are therefore intolerable.

More important in this weak dependence is the fact that the layers are essentially treated as independent because the shear surface interaction is neglected. In the actual bonded system, it is this shear force which is completely responsible for holding the system together and hence assumes the major role. In neglecting this force a major contributor to the stress levels has been left out. However, to include this shear interaction is far beyond the scope of this work and is, in fact, not treated in even the most advanced texts on the subject. The compromise solution offered here appears to be an easily understood and practical solution to the

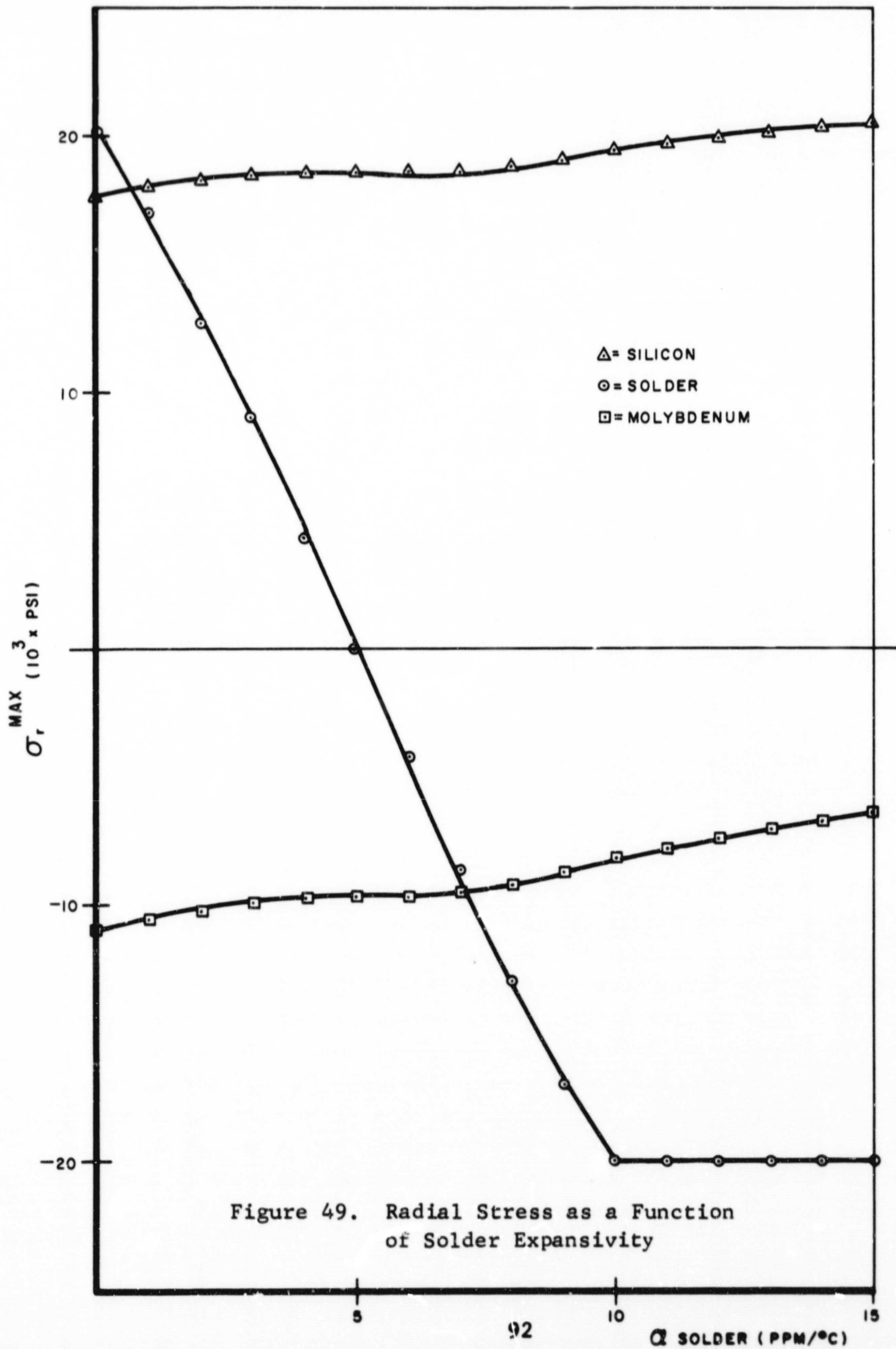


Figure 49. Radial Stress as a Function of Solder Expansivity

7641-10-8

problem. A detailed study of shear forces applied to the flat end of cylinders might be proposed for future work.

Calculations carried out for 2-inch wafers were completed, but no significant differences were encountered and therefore these are not included in the report.

2.5.9 Computer Program

The following is the program used on the GE 415 system to carry out the calculations.

01/13/69	00000AFB	THE GE-400 SERIES - FORTRAN ASA (MTPS)	SUBROUTINE	PAGE #	1	AFB	SDL6
1		SUBROUTINE A(Y,I)					
2		COMMON SRC(50),SZ(80),Z1(80),SI(80),SS(80),D(10),P(10),X1,N,ZN,L,M					
3		COMMON C6,C7,C8,H3,ER,F,GR,HR,EX,FX,GX,HX,JX,KX,PX,OX,CS,CZ,C9					
4		REAL J1,J2,J3,JA,K,JX,KX,I					
5		INTEGER 7N					
6		IF(Y=12,11+1+4					
7	1	E=-0.5					
8		OX=-0.5					
9		F=C6					
10		H=Y					
11		G=0.0					
12		JA=1.0					
13		K=C7					
14		CE=5*Y					
15		DO 3 J=1,30					
16		J3=1.0					
17		DO 2 M1=1,J					
18	2	J3=J3*M1					
19		J2=C*(2*J-1)/J3**2					
20		J1=J2*C					
21		F=E-J1*(1+2*J)*.5/(1+J)					
22		F=F+J1*(2*J+C6)					
23		OX=OX-J1*.5/(J+1.)					
24		G=G+J2*J					
25		H=H+2*J2*(C8*J+C**2)					
26		JA=JA+J1					
27	3	K=K+2*J1*(J+C9)					
28		GO TO 8					
29	4	J1=1.					
30		G=1.					
31		JA=1.					
32		E=1./Y-1.					
33		F=C6*Y					
34		H=H3*Y					
35		K=C7*Y					
36		DO 7 J=1,30					
37		J1=J1/JY/Y8.					
38		IF(J1=1,E=50)50,50.5					
39	5	J2=1.					
40		J3=1.					
41		DO 6 M1=1,J					
42		C=(2*M1-1)*2					
43		J2=J2*C					
44	6	J3=J3*(C-4.)					
45		E=E+J1*(J3/Y-J2)					
46		F=F+J1*(C6*J2+Y*J3)					
47		JA=JA+J1*J2					
48		K=K+J1*(Y*J3+C7*J2)					
49		G=G+J1*J3					
50	7	H=H+J1*(H3*J3+Y*J2)					
51	50	OX=-G/Y					
52	8	IF(1-2)10,9,10					
53	9	HR=H					
54		GR=G					


```

55 ER=E
56 ERF
57 GO TO 11
58 10 PX=C6,JA
59 KX=K
60 EX=E
61 FX=F
62 GX=G
63 HX=H
64 JX=JA
65 11 RETURN
66 END

```

```

1 SUBROUTINE A2
2 COMMON SR(80),SZ(80),ZI(80),SI(80),SS(80),D(10),P(10),X1,N,ZN,L,M
3 COMMON C6,C7,C8,B3,ER,FR,GR,HR,EX,FX,GX,HX,JX,KX,PX,QX,CS,CZ,C9
4 REAL JX,KX,L
5 INTEGER 7N
6 DS=-361802.
7 PRINT 100,X1,N
8 DO 15 J=1,ZN
9 Z=ZI(J)/L
10 N2=M-1
11 DO 14 M1=1,N2
12 IF (Z1(J)-D(M1))12,13,14
13 DC=P(M1)
14 GO TO 15
15 13 DC=.5*(P(M1)+P(M1+1))
16 GO TO 15
17 14 DC=P(M)
18 15 SSR=SR(J)-DC
19 SSI=SI(J)-DC
20 SSZ=SZ(J)-DS*7**601*(Z/602.-1./601.)*CZ
21 SSS=SS(J)-DS*7**600*(Z-1.)*CS/L
22 PRINT 101,Z1(J),SSR,SSZ,SSS,SST
23 100 FORMAT(1H1,G20.5,120)
24 101 FORMAT(5G20.6)
25 RETURN
26 END

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01/13/69	THE GE-4	THE GE-400 SERIES - FORTRAN ASA (MTPS)	PAGE # 1	THE	SDL 6
1		COMMON SR(80),SZ(80),Z1(80),ST(80),SS(80),D(10),P(10),X1,N,ZN,L,M			
2		COMMON C6,C7,C8,B3,ER,FR,GR,HR,EX,FX,GX,HX,JX,KX,PX,QX,CS,CZ,C9			
3		REAL JX,KX,L			
4		INTEGER IERM,ZN			
5		READ 200,R1,V,ZN,M			
6		READ 201,(P(N),D(N),N=1,M)			
7		L=D(M)			
8		C6=1,-2,*V			
9		C8=1,-V			
10		C9=2,-V			
11		C7=2,*C9			
12		B3=2,*C8			
13		PI=3.141592653			
14		A0=P(1)*D(1)/L			
15		DO 40 N=2,M			
16	40	A0=A0+P(N)*D(N)-D(N-1))/L			
17		C2=2./PI			
18		C5=PI/L			
19	17	READ 202,(Z1(N),N=1,ZN)			
20	18	READ 202,X1			
21		IF(X1)70,20,19			
22	19	C4=SQRT(R1/X1)			
23	20	CZ=0.			
24		CS=0.			
25		C3=EXP(C5*(X1-R1))			
26		DO 21 N=1,ZN			
27		SR(N)=A0			
28		SI(N)=A0			
29		SZ(N)=0.			
30	21	SS(N)=0.			
31		TERM=1000			
32		DO 35 N=1,TERM			
33		C1=N*C5			
34		R=C1*R1			
35		X=C1*X1			
36		IF(R-X)23,22,23			
37	22	CALL A(R,1)			
38		GO TO 31			
39	23	CALL A(R,2)			
40		CALL A(X,1)			
41		IF(R-12.)24,24,25			
42	25	IF(X-12.)28,28,26			
43	26	IF(R-X-30.)27,27,37			
44	27	CON=C4*C3**N			
45		GO TO 32			
46	28	IF(R-40.)29,29,37			
47	29	CON=EXP(-R)*SQRT(2*PI*R)			
48	30	GO TO 32			
49	31	HR=HX			
50		GR=GX			
51		FR=EX			
52		FR=FX			
53	24	CON=1.			
54	32	AN1=P(1)*SIN(C1*D(1))-P(M)*SIN(C1*D(M-1))			

01/13/69	THE GE-4	THE GE-400 SERIES - FORTRAN ASA (MTPS)	PAGE #	2	THE	SDL6
55		N2=M-1				
56		DO 41 J=2,N2				
57	41	AN1=AN1*P(J)*(SIN(C1*D(J))-SIN(C1*D(J-1)))				
58		AN=C2*CON*AN1/N/(ER*HR+FR*GR)				
59		BR=AN*(EX*HR+FX*GR)				
60		BZ=AN*(JX*HR+KX*GR)				
61		RS=AN*(GX*HR-HX*GR)				
62		BT=AN*(PX*GR+QX*HR)				
63		B1=(-1,)*N				
64		B2=C1*2				
65		DO 33 J=1,7N				
66		Z=Z1(J)*C1				
67		SR(J)=SR(J)+BR*COS(Z)				
68		SZ(J)=SZ(J)+BZ*COS(Z)				
69		SS(J)=SS(J)+RS*SIN(Z)				
70	33	SI(J)=SI(J)+B1*COS(Z)				
71		CZ=CZ+B1*BZ				
72		CS=CS-B1*BS/C1				
73		IF(N-TERM)35,34,35				
74	34	CALL A2				
75		TERM=TERM+1000				
76		IF(ITERM=6000)35,18,18				
77	35	CONTINUE				
78	37	CALL A2				
79	38	GO TO 18				
80	200	FORMAT(2G20.6,2I10)				
81	201	FORMAT(2G20.6)				
82	202	FORMAT(2G20.6)				
83	70	CALL EXIT				
84		END				

SECTION III

3.0 CONCLUSIONS

This program has shown that the bonding of large area wafers to heat sinks is a much more difficult problem than its counterpart on a small scale. Current techniques, i.e., eutectic soldering and ultrasonic die bonding, appear to be impractical since the former has a void problem which is amplified on a large scale, and the latter requires impossible forces when a reasonably large area die is used. In addition, many eutectic solders are hard and very strong. This, coupled with the fact that they have relatively large expansivities, makes wafer cracking a major problem.

Of the five modes of bonding investigated during the program, three show a great deal of promise; Diffusion Bonding, Amalgam Bonding, and Anodic Bonding.

Liquid state diffusion bonding has been shown to produce reliable bonds of wafers up to two inches in diameter to molybdenum heat sinks. These bonds are uniform, resistant to thermal shock, and do not affect device performance. Voids still present a major problem but we have shown that they can be eliminated if care is taken in selecting the materials and procedures. Mechanical stability (i.e., freedom from wafer cracking, and solder embrittlement), can be achieved by bonding high quality wafers with solder compositions selected to reach equilibrium with the majority of the solder in a solid solution phase. These will possess all the necessary qualities of a good bond-uniformity, good conductivity and mechanical stability. It is noteworthy that the presence of indium in the solder appears to be the key to achieving the desired performance.

Solid state diffusion bonds between 1-inch and 2-inch wafers and single heat sinks have not been obtained, although inter-wafer bonds and double heat sink bonds are of excellent quality. This is not to say that the solid-solid bonding method is not useful. It still provides reliability with low thermal resistance, in cases where ultrasonic bonders with sufficient forces for deformation (i.e., the die is less than 100 x 100 square mils) can be utilized, or large area diode devices of high power are produced.

The amalgam bonding method can be used just as diffusion bonding and presents an area where future studies can be made.

The use of plastic solders has been shown to be severely limited, due to poor compatibility in expansivity and low thermal conductivity.

The anodic bonding scheme appears to present an attractive alternative in cases where the device power dissipation is low. The bonds are strong as well as inexpensive to make, and the entire process seems readily adaptable to a production process, especially in the case where one can bond to a glazed alumina or similarly structured substrate.

Investigations into this and related processes should certainly be a prime area for future work.

The program has also generated much useful data on the solders presently used in the semiconductor industry. Our results indicate that in the case of large area and high power dissipation, where expansivity matching and good thermal conductivity are a necessity, one must look toward new solder systems. When our data on silver-indium is added to this, it can readily be seen that the solid-solution solder should be the ultimate in bonding material.

Whether achieved by the schemes proposed herein or by some completely different method, it is only in the metallic solid solution that we can find all the properties characteristic of a good bond.

The computational phase of the program has shown that the problem of residual stress in the bonded system is one of great importance. Results indicate that the stress levels can be significant enough to cause a change in device parameters, as well as degrading the mechanical stability of the entire bonded system. Although we have solved a problem not exactly identical to the "real-world" wafer-to-heat sink bond; we feel that the results obtained make a valuable contribution to the understanding of bonds and bonding materials.

3.1 RECOMMENDATIONS FOR FUTURE WORK

The program has also indicated some areas where future work could bear fruit. It has only begun to establish the systems wherein diffusion bonding and its relatives can be useful. The wealth of metallurgical systems, particularly where the alloys are liquid at near room temperature, have barely been touched. As the mechanisms of the anodic bond become better understood, it should yield more applications than the very few possible now.

Our computer calculation indicates that some useful results can be achieved, and future programs to solve the problem of the sheared cylinder should provide a more detailed, and more accurate, look at the multilayer bond.

This program has provided some inroads of information into a problem which will be of prime concern to the microelectronics industry in the near future; that of large area heat

sinking. The problem certainly will take further effort for more refined solutions, but enough is now known to dictate approaches that can be followed in a practical situation.

SECTION IV

4.0 REFERENCES

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