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HIGH TEMPERATURE SOLAR CELL CONTACTS

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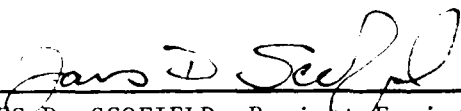
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<p>Gallium arsenide solar cells may be subjected to extreme temperature excursions as high as 600°C during processing steps and while operating in space orbits. To prevent solar cell failure during fabrication and its operating life, the electrical contacts to the active semiconductor material must remain electrically and chemically stable during these high temperature excursions.</p> <p>The objective of this effort is to develop an electrical contact material to the gallium arsenide solar cell which will survive temperatures up to 600°C (873K) for periods up to 15 minutes.</p> <p>During this contracting period a thermodynamic phase equilibrium computer model was developed which calculates the liquidus and solidus phase boundaries of metal-Ga-As systems of interest to determine their potential high temperature stability.</p>						
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1. INTRODUCTION

The University of Dayton has conducted research for the purpose of developing high temperature electrical contacts for gallium arsenide solar cells.

1.1 Statement of the Problem

Gallium arsenide solar cells may be subjected to temperatures as high as 600°C during processing steps and to high-temperature thermal excursions while operating in space environments. To prevent failure of the solar cell during its preparation and operating life, the electrical contacts to the active material must remain electrically and chemically stable during these high-temperature excursions.

1.2 Objective

The objective of the research effort was to develop an electrical contact material to the gallium arsenide solar cell which would survive at temperatures up to 600°C (873K) for time intervals on the order of 15 minutes.

The temperature constitution phase diagrams of selected binary alloy systems were reviewed as part of our investigation of the high temperature stability of electrical contacts to gallium arsenide solar cells. The phase diagram is a graphic representation of the alloy phase or phases which are in thermodynamic equilibrium as a function of the temperature and chemical composition of the system. The data contained in the phase diagram which are of immediate interest for evaluating potential contact materials are the composition of the alloy phase or phases which can coexist with gallium arsenide and the presence of any phase transformations. Thus by reviewing the pertinent phase diagrams, the likelihood of chemical reactions between the electrical contact material and the gallium arsenide solar cells can be determined.

The binary systems which were reviewed contained either gallium or arsenic as one of the constituents, and either copper, silver, gold, or aluminum as the second constituent. Copper, silver, gold, and aluminum were selected because these metals could be used as electrical contacts. Attention was also focussed on materials which could maintain a physical separation between the gallium arsenide solar cells and the electrical contact material. The elements beryllium, boron, and

carbon were reviewed to determine their usefulness as a buffer layer between the gallium arsenide and the electrical contact metal.

2. PHASE DIAGRAM REVIEW

The ternary phase diagrams containing gallium and arsenic as two of the constituents, and either copper, silver, or gold as the third constituent were reviewed. The phases and the phase transformations which have been reported¹⁻⁴ in these binary and ternary systems are summarized in the following paragraphs.

2.1 Binary Phase Diagram Review

The principal liquid-solid transformations which have been reported in these systems are eutectic transformations in which a liquid phase transforms into two solid phases of different compositions, and the melting of intermediate phase compounds either with or without a change in their chemical composition. The liquid-solid transformations are briefly summarized in the following paragraphs.

Silver-Arsenic System (Ag-As)

One compound was reported in the silver arsenic system. The compound has a composition of 90 atomic percent silver and is stable only at higher temperatures. There is uncertainty as to the exact temperature interval over which the compound is stable; Hansen¹ reports the interval to be 374 to 595°C, while Elliott² reports the interval to be 446 to 582°C. This compound undergoes a peritectic transformation at 595°C into a silver solid solution saturated with arsenic and a liquid phase containing 78.5 atomic percent silver. Although silver is not soluble in elemental arsenic, arsenic is soluble in solid silver, reaching a maximum solubility of 8.8 atomic percent arsenic at 595°C. There is an eutectic transformation at 540°C between elemental arsenic and the silver-rich compound. The eutectic liquid phase is at 74.7 atomic percent silver.

Silver-Boron System (Ag-B)

Early studies¹ reported that boron was insoluble in molten silver at 1500°C under a hydrogen atmosphere. More recent research concluded that boron is slightly soluble in molten silver. A silver-boron compound, Ag₂B, has been synthesized, but no other thermal property data were reported.

Silver-Beryllium System (Ag-Be)

The binary system contains an eutectic comprised of 89.5 atomic percent silver at 881°C. Two intermediate compounds have been reported to be stable at temperatures greater than 760°C.¹ One of these compounds, the delta phase, has a beryllium composition of 74 atomic percent, the balance being silver, and this compound is stable over a temperature interval of 850 to 1010°C. The second phase is designated as the gamma phase and has a beryllium composition of 63 atomic percent. The gamma phase is stable over a temperature interval of 760 to 860°C. Below 760°C, elemental solid beryllium coexists with elemental solid silver.

Silver-Carbon System (Ag-C)

The solubility of carbon in molten silver has been reported¹ to be 0.0012 weight percent at 1660°C. The compound, Ag₂C₂, has been reported to be formed by chemical means³. This is contrary to the earlier research which reported that the entire carbon content of the silver-carbon liquid phase crystallizes as graphite.

Silver-Gallium System (Ag-Ga)

There is an eutectic transformation at 25°C between elemental gallium and a silver gallium compound. The eutectic point is at a composition of 97 atomic percent gallium. The silver gallium compound contains 60 atomic percent gallium and undergoes a peritectic transformation at 326°C into a liquid phase containing 82 atomic percent gallium and a second compound. This second compound contains 60 atomic percent silver and transforms into a high temperature modification at 425°C. This high temperature phase undergoes a peritectic transformation at 611°C into a solid silver phase saturated with 18.7 atomic percent gallium and a liquid phase containing 72 atomic percent silver.

The liquid phase boundary in the silver-gallium system which exists below 500°C extends from elemental gallium to compositions containing more than 50 atomic percent silver.

Aluminum-Arsenic System (Al-As)

This phase diagram has not been reported¹⁻³. The compound AlAs has been reported to have a melting point which is pressure sensitive and has a maximum at 1740°C at a pressure of 1 atmosphere.

Aluminum-Boron System (Al-B)

Two intermediate compounds, AlB₂ and AlB₁₂, have been reported in the aluminum boron system. These two compounds transform by peritectic reactions. The compound AlB₂ transforms at 975°C into an aluminum-rich liquid phase and the compound AlB₁₂. The compound AlB₁₂ transforms at 2070°C into an aluminum-boron liquid phase and elemental boron. There is an eutectic transformation at 659.7°C and at a composition of 0.55 atomic percent boron.

Aluminum-Beryllium System (Al-Be)

The aluminum beryllium system is a simple eutectic system with the eutectic transformation at 645°C. The eutectic point is located at a composition of 2.5 atomic percent beryllium. No reaction was found between aluminum and beryllium after annealing clamped specimens for 8.5 days at 600°C.

Aluminum-Carbon System (Al-C)

The phase diagram has not been reported¹⁻³. However, the existence of an intermediate phase, Al₄C₃, has been repeatedly verified¹⁻³. Additionally, carbon has been reported to be slightly soluble in both solid and liquid phases of aluminum.

Aluminum-Gallium System (Al-Ga)

The phase diagram of the aluminum gallium system is depicted as a simple eutectic system¹. The eutectic transformation has been reported at a temperature of 26.6°C and at a composition of 2.5 atomic percent aluminum³. The

solid solubility of gallium in aluminum has been reported to be 8.8 atomic percent gallium at the eutectic temperature and decreasing in value as the temperature is increased.

Arsenic-Gold System (As-Au)

Hansen¹ reported an eutectic reaction at 630°C and at a composition of 50 atomic percent arsenic. The only solid phases observed to be present are gold and arsenic, each with a slight amount of mutual solid solubility.

Arsenic-Boron System (As-B)

Three compounds have been reported in this system. The compound AsB formed by interdiffusion of the two elemental solid substances is stable to 920°C in the presence of an arsenic vapor. The other two compounds have compositions corresponding to AsB₆ and As₂B₁₃. No other thermal property data were reported on these compounds.

Arsenic-Beryllium System (As-Be)

The only research findings² on this binary system reported the formation of a compound with no further elaboration.

Arsenic-Carbon System (As-C)

Although carbon has been reported¹ to be insoluble in arsenic at its sublimation point, presumably at a pressure of one atmosphere, there is a report³ of the formation of the compound AsC₃ by chemical means.

Arsenic-Copper System (As-Cu)

There are three compounds in this binary system. The compound Cu₈As decomposes at 480°C into solid copper saturated with arsenic and the compound Cu₃As, which melts without a change in composition at 827°C. The third compound, Cu₅As₂, is stable only in the interval 300 to 709°C. At 300°C, this compound transforms into solid arsenic and the compound Cu₃As. At 709°C, this compound undergoes a peritectic transformation into a liquid phase containing 33 atomic percent arsenic and the compound Cu₃As. There are two eutectic reactions

in the system, one of which occurs between elemental copper and the compound Cu_3As at 685°C . The second eutectic reaction occurs between the compound Cu_5As and elemental arsenic at 600°C .

Arsenic-Gallium System (As-Ga)

There is one intermediate solid phase, the compound gallium arsenide, whose melting point is reported to be 1238°C . There are two eutectic transformations, one at 99.99% gallium and at 29.5°C , and the other at 810°C and a pressure of 30 atmospheres at a composition of 98 atomic percent arsenic. These two eutectic transformations are between gallium arsenide and the pure elements, respectively.

Gold-Boron System (Au-B)

The preparation of the compound AuB_2 , has been reported². Boron has been reported to be slightly soluble in solid elemental gold. No other thermal property data were reported.

Gold-Beryllium System (Au-Be)

Four compounds have been reported in the gold-rich portion of the phase diagram¹. Two of the compounds, BeAu_3 and Be_3Au_4 , have peritectic reactions occurring at 595°C and 610°C , respectively. The other two compounds, BeAu_2 and BeAu , melt congruently at 645°C and 730° , respectively. In addition, there are two eutectic transformations; one occurs at 580°C and at a composition of 80 atomic gold, and the other occurs at 602°C and at a composition of 60 atomic percent gold.

Gold-Carbon System (Au-C)

An early research investigation concluded that carbon was soluble to the extent of 0.3 weight percent, at the normal boiling point of gold, and that the carbon crystallizes as graphite from the melt on cooling¹. A more recent investigation reported the synthesis of the compound Au_2C_2 , by chemical means³.

Gold-Gallium System (Au-Ga)

There are two congruently melting compounds in this system. The compound AuGa_2 melts at 492°C and the compound AuGa melts at 461°C .¹ In addition to these two compounds, there are several peritectic compounds in the gold-rich portion of the phase diagram. There are three eutectic compositions reported; one at 99.99 atomic percent gallium and at 30°C between elemental solid gallium and AuGa_2 ; a second eutectic transformation occurs at a temperature of 451°C between the compounds AuGa_2 and AuGa ; the third eutectic occurs at 341°C and a composition of 67 atomic percent gold between AuGa and a gold-rich peritectic compound. There is a phase transformation recorded at 275°C which evidently is a solid state transformation of this peritectic compound into a modification which is stable at room temperature.

Boron-Copper System (B-Cu)

An eutectic transformation has been reported at 1060°C and at a composition of 89.3 atomic percent copper. In addition, a boron-rich compound, B_{22}Cu , has been reported¹, but there were no other thermal data available. In view of the high melting points of the two elemental constituents and the value for the eutectic temperature, the melting point of this compound is expected to be greater than 1060°C .

Boron-Gallium System (B-Ga)

A compound, B_{12}Ga , was synthesized by sintering the elements at 1200°C in vacuo². No other thermal data were available on this system.

Beryllium-Copper System (Be-Cu)

The beryllium copper binary system contains several intermediate phases. The compound Be_3Cu melts at 1239°C . A second intermediate phase forms a solid solution with a solubility range between 76.4 and 50 atomic percent copper and melts at $\sim 860^\circ\text{C}$. Both of the elemental solids have some mutual solid solubility. At 600°C , solid copper dissolves 10 atomic percent beryllium. At the same temperature, the solid solubility limit of copper in elemental beryllium is 5 atomic percent.

Beryllium-Gallium System (Be-Ga)

The principal feature of the beryllium gallium system is the monotectic reaction at 1250°C.² At this temperature the elemental solid, Be, reacts with a gallium-rich liquid phase to form a beryllium-rich liquid phase.

Carbon-Copper System (C-Cu)

The compound C_2Cu_2 , has been reported to be synthesized by chemical means³. Carbon is sparingly soluble in liquid Cu.²

Carbon-Gallium System (C-Ga)

There are no data available for this system.

Copper-Gallium System (Cu-Ga)

The copper gallium system is characterized by an eutectic transformation and four intermediate peritectic compounds. The eutectic transformation occurs at 29.6°C and at a composition of 99.9 atomic percent gallium. The peritectic compound $CuGa_2$ transforms at 254°C into a liquid phase that has a composition of 96 atomic percent gallium and a second peritectic compound. This second peritectic compound undergoes a peritectic transformation at 485°C into a liquid phase containing 73 atomic percent gallium and a third peritectic compound. This third alloy has a peritectic transformation at 836°C into a liquid phase containing 31 atomic percent gallium and a fourth peritectic compound. This fourth compound undergoes a peritectic transformation at 915°C into a liquid phase containing 21 atomic percent gallium and a solid copper phase which is saturated with gallium.

2.2 Ternary Phase Diagram Review

The phase diagrams for the ternary systems containing gallium and arsenic, and one of the Group 1-B elements, copper, silver, and gold, were reviewed. Phase equilibria studies in these ternary systems have been reported by Panish⁴. The phase transformations reported in these systems are summarized in the following paragraphs.

Gallium-Arsenic-Copper System (Ga-As-Cu)

Panish observed an eutectic reaction at 594°C among the solid phases, gallium arsenide, and the compound Cu_3As . A second eutectic reaction was observed at 667°C among the three compounds GaAs , Ga_4Cu_9 , and AsCu_3 . The compositions of these eutectic compositions have not been determined with any precision.

Gallium-Arsenic-Silver System (Ga-As-Ag)

The phase equilibria in the ternary system Ga-As-Cu have been investigated by Panish. A ternary eutectic reaction was observed at 532°C in which GaAs , elemental arsenic, and an intermediate silver-arsenic alloy were precipitated.

The phase transformations for compositions between gallium arsenide and silver resemble those of a pseudo-binary eutectic system. The only phases observed to precipitate from the liquid phase for compositions less than 82 atomic percent silver were pure gallium arsenide and silver. For higher silver compositions, the temperatures and compositions of the solid silver alloys precipitated from the liquid phase are slightly different from those expected from a true pseudo-binary system.

A liquid-solid transformation was observed to occur along a composition line fixed at 50 atomic percent gallium. This transformation occurs at 285°C and is related to the peritectic transformation which occurs in the related Ag-Ga binary system at 325°C. The solid phases present after cooling were gallium arsenide, a Ag-Ga alloy containing equal amounts of silver and gallium, and a silver phase. There is, of course, the eutectic transformation described above in the Ag-Ga binary system.

Gallium-Arsenic-Gold System (Ga-As-Au)

Panish conducted an experimental study of this alloy system. A ternary eutectic reaction was observed at 580°C among the three solid phases, gold, arsenic, and gallium arsenide. This ternary eutectic transformation is related to the binary eutectic reaction reported in the As-Au binary system. He reports an eutectic reaction between the compounds GaAs and GaAu at 440°C. The temperature of this

transformation is uncertain due to supercooling of the specimens during the cooling cycles. (See also the eutectic reactions discussed above in the Au-Ga and the As-Au binary systems.)

2.3 Phase Diagram Review - Summary and Recommendations

The phase equilibria in ternary alloy systems containing gallium, arsenic, and one of the elements, copper, silver, and gold, have been reviewed with an emphasis on identification of those phase transformations which can be expected to cause degradation of the electrical contact to the gallium arsenide. In each of the three ternary systems, liquid-solid phase transformations were observed at temperatures below 600°C.

The application of either copper, silver, or gold as the electrical contact to gallium arsenide at elevated temperatures will require a barrier layer whose function is to maintain physical separation between the gallium arsenide and the electrical contact. The elements, boron, beryllium, and carbon were considered for this purpose. As a result of a review of the phase diagrams of these materials with either gallium or arsenic, the use of beryllium to stabilize the electrical contact is not recommended if gold is used as the electrical contact, since liquid-solid reactions have been reported below 600°C in the Au-Be system. Beryllium is also a very toxic substance, and is therefore not recommended for use in this application. Based on the available information, boron and carbon are recommended for further study. Compound barrier layers such as TiN, TiWN, and TiW are also recommended for further study.

3. ANALYTICAL MODELING OF THE PHASE DIAGRAM

In contrast to the availability of binary phase diagrams, relatively few ternary phase diagrams have been reported which contain gallium and arsenic as two of the three elemental constituents. The effort required to determine a ternary phase diagram places a practical limit on the number of systems which can be experimentally investigated. To overcome this limitation, the development of a mathematical model was initiated which will calculate the phase boundaries of ternary systems.

In the present analysis, the free energy of the binary and ternary phases are

represented by the regular solution theory which models the free energy of a binary alloy by a single parameter that characterizes the chemical reaction between elemental constituents. In the case of ternary alloys, the regular solution parameter is a linear combination of the parameters describing the three binary systems that are subsets of the ternary system. These binary parameters can be calculated from a single datum point of the temperature and composition of the liquidus boundary of the pertinent binary phase diagrams.

The procedure for developing the analytical expressions for the liquidus and solidus boundaries consists of the following steps:

1. Apply the principle of heterogeneous phase equilibrium which states that the partial molal free energy of each of the elemental constituents in all of the separate phases must be equal at equilibrium.
2. Express the partial molal free energy terms of each of the elemental constituents as functions of the standard state free energy of the pure elements, the activity coefficients, the mole fractions, and the absolute temperature.
3. Express the difference between the standard state free energies of the liquid and solid states of each of the elements in terms of their enthalpies of fusion and melting temperatures.
4. Apply the regular solution model of alloying behavior to obtain expressions for the activity coefficients of each of the constituents.
5. Utilize the existing phase boundaries in the binary systems to calculate the parameters of the regular solution model. These steps lead to the development of analytical expressions for the phase boundaries of the phase diagram.

3.1 Results

The analytical expressions for the phase boundaries of two types of binary systems have been developed. A FORTRAN-77 computer code was developed and tested which calculates the phase boundaries for alloy systems containing a single intermediate compound. The gallium-arsenic alloy system belongs to this family of phase diagrams. A second computer code was developed and tested which calculates the phase boundaries of the simple binary eutectic alloy system. The gallium-zinc alloy system is an example of this kind of system.

The analytical expressions for two types of phase boundaries for ternary systems have been developed. The ternary liquidus phase boundary which is in equilibrium with a binary compound was modeled, and the equations describing the ternary liquidus boundary which is in equilibrium with the terminal ternary solid phase were developed. The ternary alloy systems containing gallium and arsenic as two of the three elemental constituents have these types of liquidus boundaries.

Binary Phase Diagrams

A FORTRAN-77 computer code was developed which utilizes the existing temperature and composition data of the liquidus and solidus boundaries for binary systems to calculate the parameters of the regular solution model. This code was applied to the gallium arsenic system to calculate the regular solution parameter for the liquid phase. Three reports have been published on the melting temperature and the heat of fusion for gallium arsenide⁵⁻⁷. These data were combined with data points from the binary phase diagram of the gallium arsenide system to calculate the values of the binary liquid parameter. The data necessary for the calculations and the results are presented in Table 1. The values of the regular solution parameter for the binary liquid phase are plotted as a function of temperature, and these data were fitted by the least squares method to a linear function of the temperature for the three sets of data. The results of these calculations for the binary regular solution liquid parameter are presented in Figure 1.

The liquid phase boundary which is in equilibrium with the solid compound of gallium arsenide was calculated over an extended range of the

TABLE 1
DATA AND RESULTS FOR GALLIUM ARSENIDE

a. Values for the melting temperature and heat of fusion of gallium arsenide

Melting Point (deg K)	Heat of Fusion (cal/gm-at)	Reference
1518.0	+10500	5
1513.0	+12590	6
1513.5	+13500	7

b. Data for the intercept and slope of the binary liquid parameter

Intercept (cal/gm-at)	Slope (cal/gm-at/K)
-3.760E+03	0.4200E+01
-1.670E+03	0.2795E+01
-0.759E+03	0.2197E+01

c. Temperature and composition of the binary liquidus boundary

Temp (degK)	Mole Fraction of the Liquidus Boundary			
	Ref. 3	Ref. 5	Ref. 6	Ref. 7
718	0.00004	0.00014	0.00002	0.00001
783	0.0002	0.00042	0.00009	0.00004
858	0.001	0.00123	0.00034	0.00019
953	0.005	0.00379	0.00140	0.00089
1063	0.02	0.01093	0.00535	0.00386
1153	0.05	0.02274	0.01343	0.01051
1238	0.1	0.04226	0.02897	0.02419

GaAs

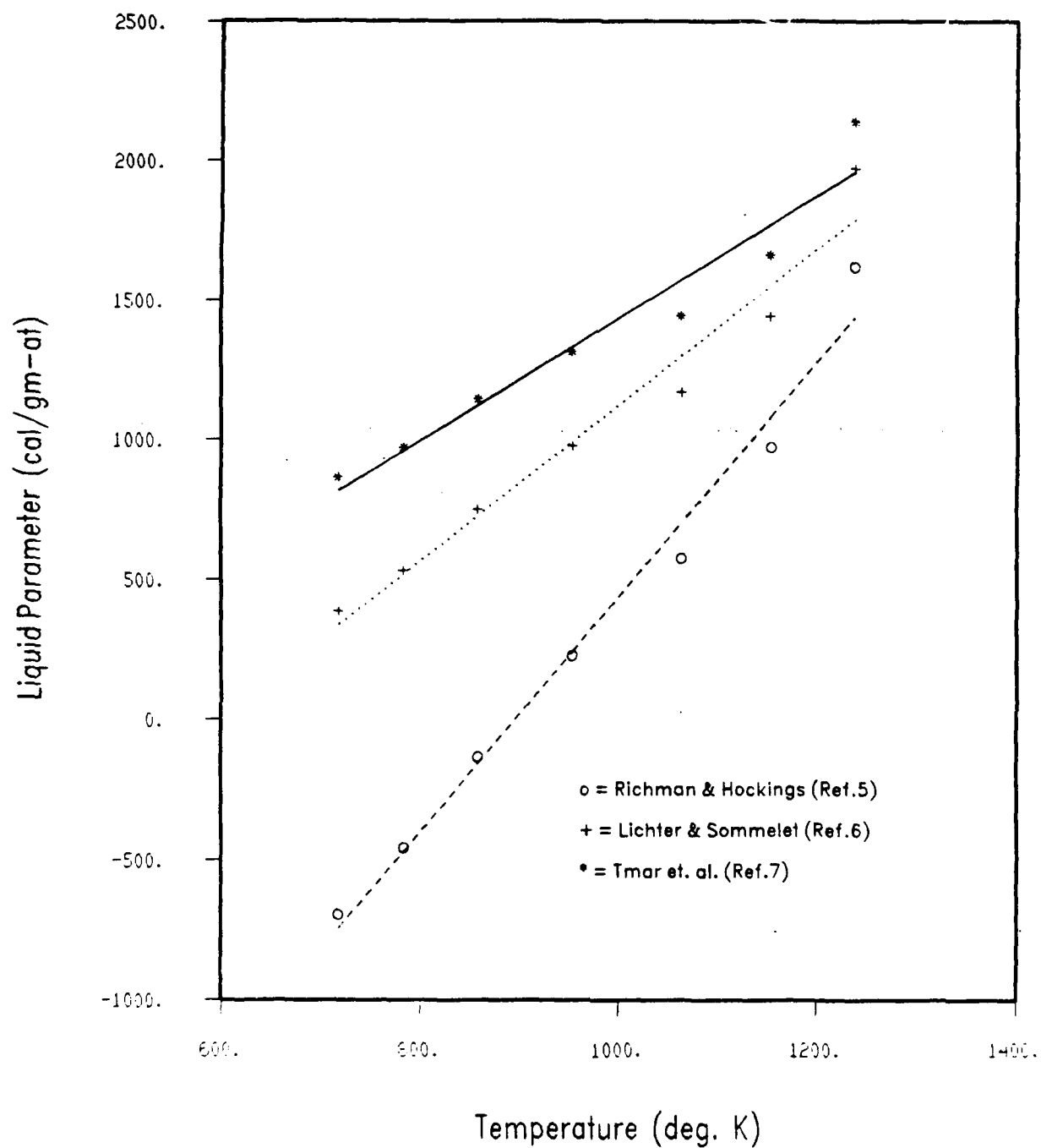


Figure 1. The plot of the binary regular solution parameter as a function of temperature for the gallium-arsenic system.

temperature and composition. The results of these calculations are presented in Figure 2. A comparison of the values for the liquidus boundaries for the three sets of data showed a slight variation in the location of the liquidus boundary.

The results of calculations for the gallium zinc alloy system are presented in Figure 3. The eutectic point, e_1 , is displaced toward the lower melting element, gallium, because of the large difference between the melting points of gallium and zinc. The liquidus and solidus phase boundaries which terminate on elemental gallium (on the right hand side of the plot) are just barely discernible. The behavior of the solidus boundary which terminates on the elemental zinc solid phase on the left hand side of the plot exhibits retrograde solubility. What this means is that the solubility of gallium in the solid zinc phase increases as the temperature decreases from the melting point of zinc. At a temperature between the melting point and the eutectic temperature, the solubility of gallium in the solid zinc phase reaches a maximum value and then decreases as the temperature continues to decrease. The calculated phase diagram for this system is in excellent agreement with the published experimental results.

Ternary Phase Diagrams

A FORTRAN-77 computer code was developed which calculates the temperature and composition of the ternary liquid phase which is in thermodynamic equilibrium with an intermediate binary compound. A plot of a test of the code is presented in Figure 4. The data for the gallium arsenide binary system were used to generate the phase boundary presented in this figure. The edges of the triangular plot represent the three binary systems which are subsets of the ternary system. The phase equilibria and the ternary liquidus boundary shown in this figure is at a temperature of 1300K. The area between this boundary and the horizontal axis represents the compositions at 1300K which consist of the ternary liquid phase and the solid gallium arsenide phase. The area between the liquidus boundary and the two diagonal axes represents the compositions at 1300K which will consist of a single homogeneous liquid phase.

A second ternary computer code which models the liquidus and solidus phase boundaries that terminate on one of the elemental constituents was developed and tested. A plot of the silver-rich corner of the ternary system

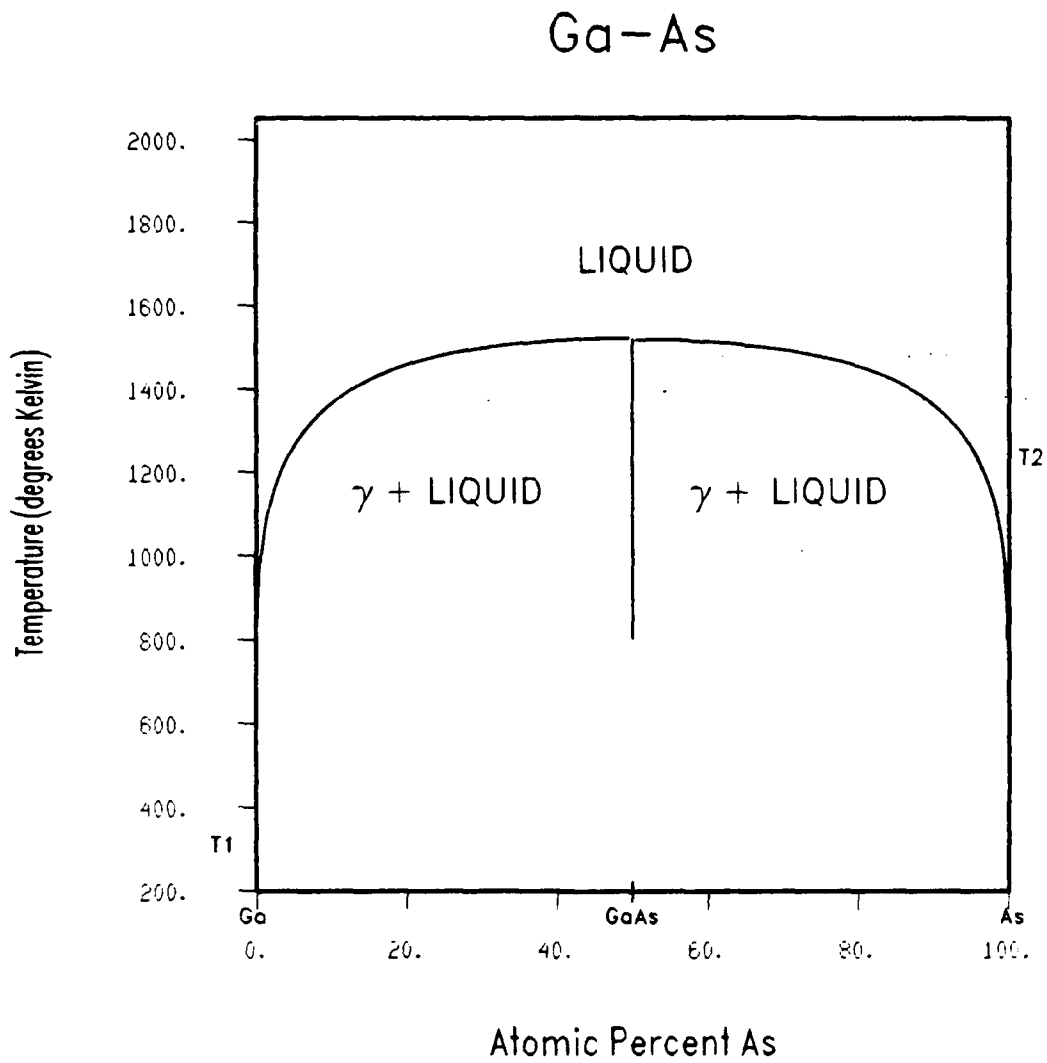


Figure 2. The calculated binary liquidus boundary which is in thermodynamic equilibrium with the compound, gallium-arsenide.

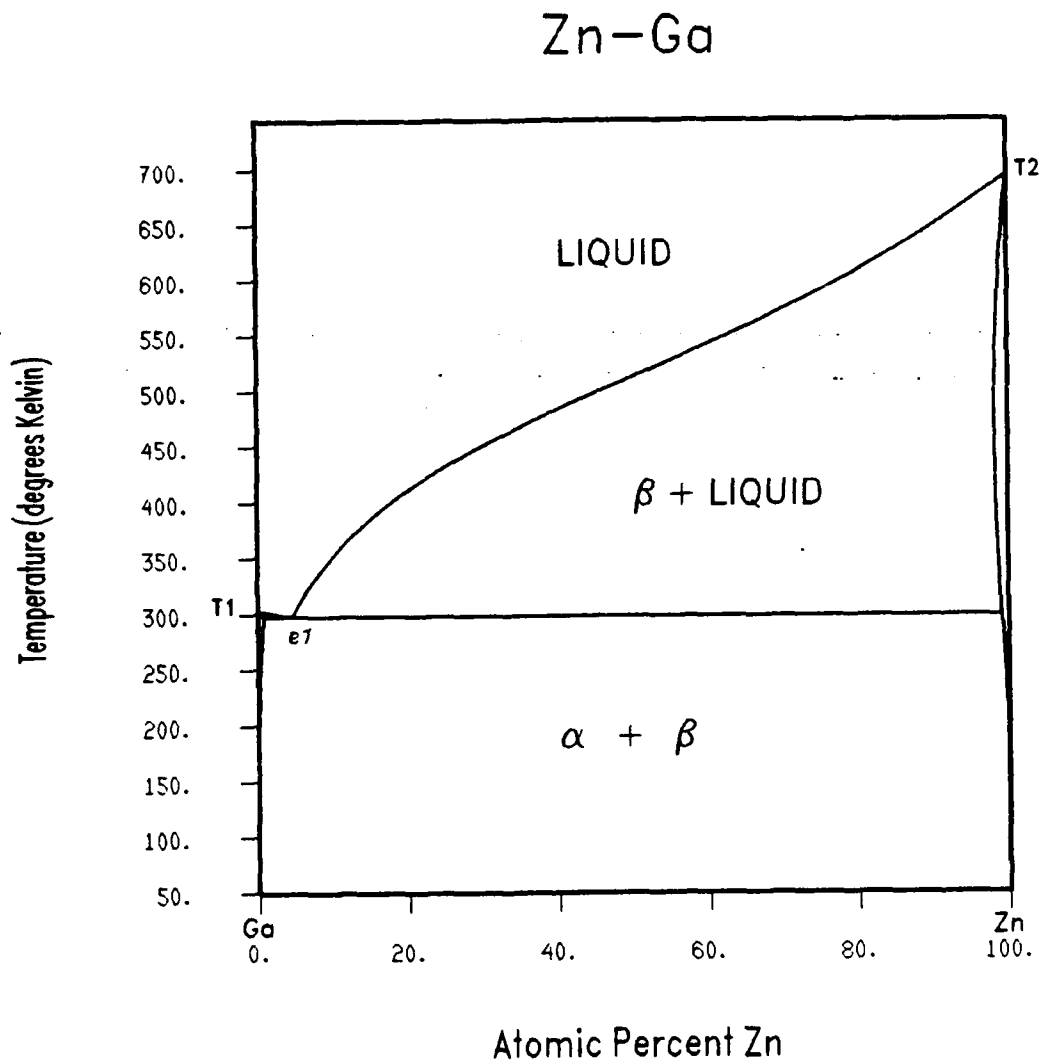


Figure 3. The calculated liquidus and solidus phase boundaries for the gallium-zinc system.

GaAsAg

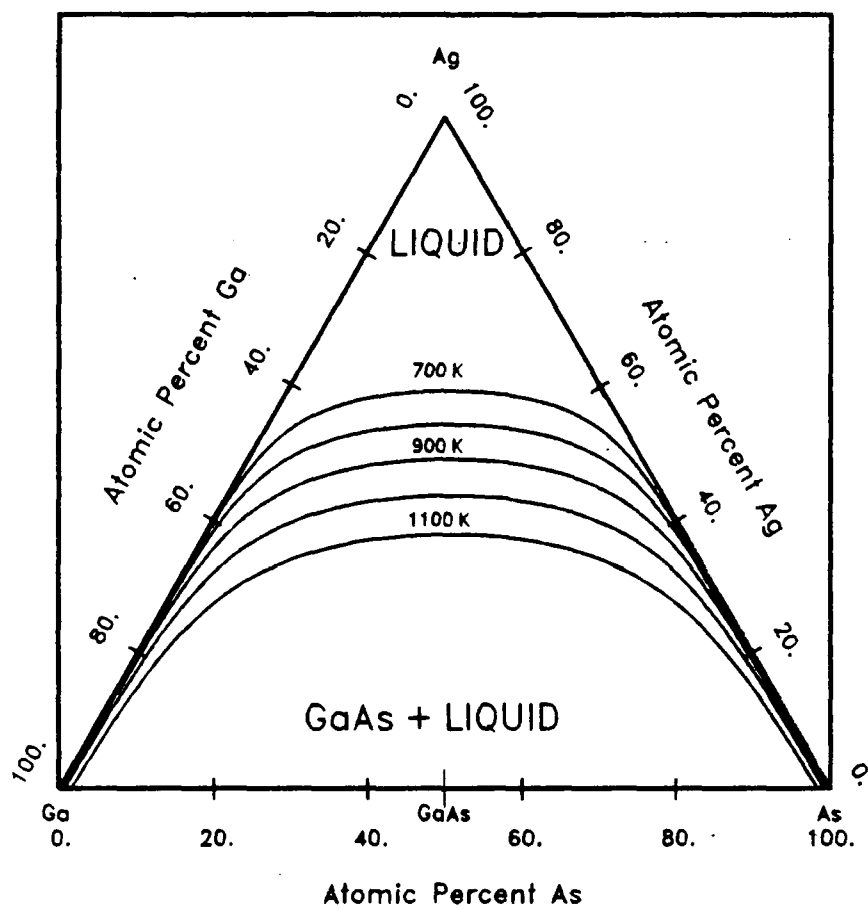


Figure 4. The calculated ternary liquidus boundary between the ternary Ag-Ga-As liquid phase and the gallium arsenide compound at temperatures of 700, 800, 900, 1000, and 1100K.

containing silver, gallium, and arsenic is presented in Figures 5a and 5b. The plot in Figure 5a depicts the liquidus and solidus boundaries at 800K. The phase 'alpha' represents the terminal silver solubility region. The solidus boundary represents the maximum solubility of gallium and arsenic in solid silver at this temperature. The liquid phase represents the compositions for which the silver, gallium, and arsenic will form a liquid phase at this temperature. The two-phase region which is labeled 'alpha plus liquid' represents those compositions for which the liquid and the alpha phase will coexist at this temperature. The plot presented in Figure 5b shows the tie lines between the liquidus and solidus boundaries. The tie lines connect the precise compositions of the alpha and liquid phases which are in equilibrium.

The combination of the results from these two ternary codes can be utilized to determine the intersection of the ternary liquidus phase boundaries, the temperature of the liquid solid transformations, and the composition of the silver alloy which is in equilibrium with the gallium arsenide compound.

4. SUMMARY

The thermal stability of copper, silver, and gold electrical contacts to gallium arsenide was assessed by reviewing existing binary and ternary temperature constitution phase diagrams. The ternary phase diagrams, which contain gallium and arsenic as two of the elemental constituents, and either copper, silver, or gold as the third elemental constituent, have liquid-solid transformations below 600°C. The use of either copper, silver, or gold as an electrical contact to gallium arsenide at 600°C will require an intermediate layer to maintain a physical separation between the active material and the electrical contact. The elements beryllium, boron, and carbon were considered for this purpose. As a result of a review of the phase diagrams of these materials with either gallium or arsenic, the use of beryllium to stabilize the electrical contact is not recommended if gold is used as the electrical contact, since liquid-solid reactions have been reported below 600°C in the Au-Be system. Based on the available information, boron and carbon are recommended for further investigations as potential buffer layers between gallium arsenide and either copper, silver, or gold. Beryllium is also a very toxic substance, and is therefore not recommended for use in this application. Based on the available

AgGaAs

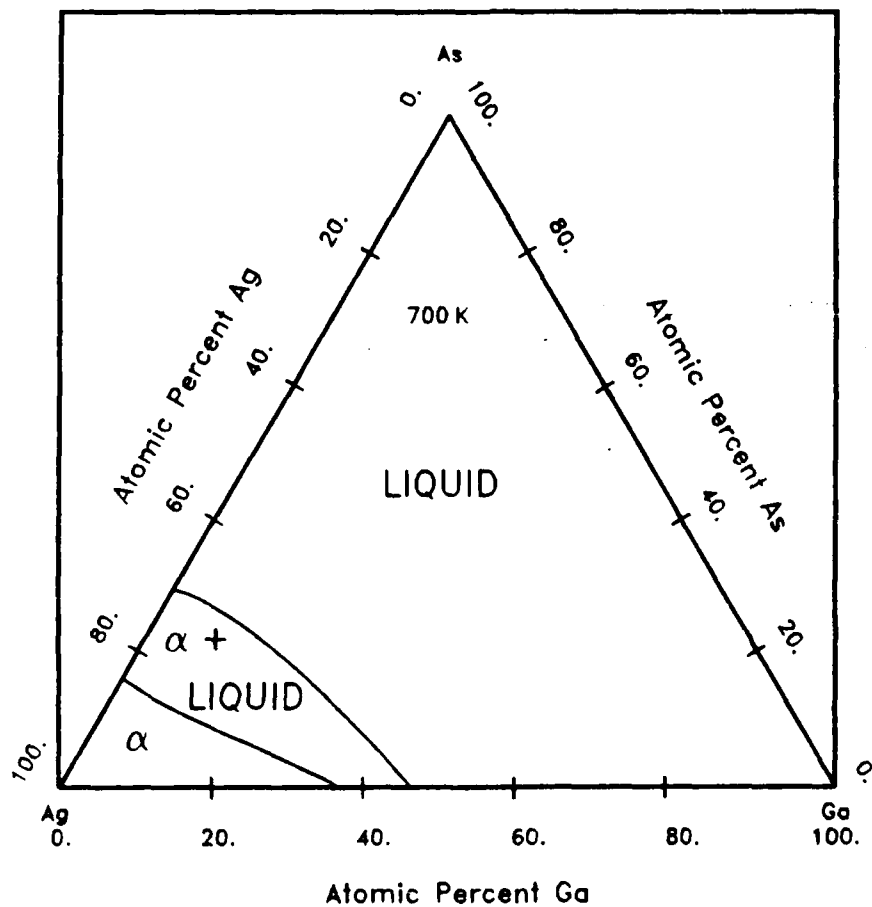


Figure 5a. The calculated ternary liquidus and solidus boundaries in the silver gallium arsenic (Ag-Ga-As) system for the silver-rich terminal solid solubility region. Shown are the ternary liquid phase, the solid silver alloy phase, and the two phase region at 700K.

AgGaAs

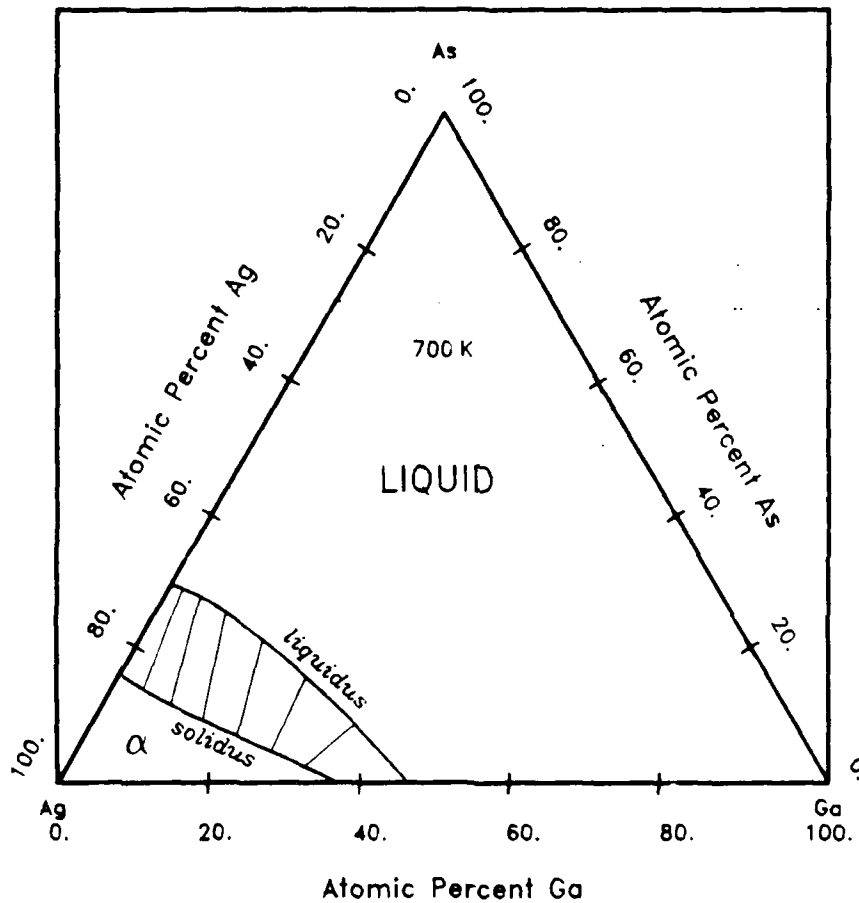


Figure 5b. The calculated ternary liquidus and solidus boundaries in the silver gallium arsenic (Ag-Ga-As) system for the silver-rich terminal solid solubility region. Shown are the ternary liquid phase, the solid ternary silver alloy phase, and the tie lines which connect the compositions of the ternary liquid phase and the ternary solid silver alloy which are in equilibrium at 700K.

information, boron and carbon are recommended for further study. Compound barrier layers such as TiN, TiWN, and TiW are also recommended for further study.

An analytical model of the phase boundaries for ternary alloy systems containing gallium and arsenic as two of the elemental constituents was developed to enable the assessment of liquid-solid transformations between the gallium arsenide and a third element. The function of this third element is to maintain a physical separation between the gallium arsenide and the electrical contact. A computer code has been developed and tested which calculates the ternary liquid composition which is in equilibrium with gallium arsenide. A second computer code was developed which models the composition of the ternary liquid phase which is in equilibrium with an elemental substance. The results from these models can be utilized to determine the intersection of the ternary liquidus boundaries. The intersections represent the temperature and composition of the liquid solid transformations which will be utilized to determine the compositions of the alloy contact which are in equilibrium with the gallium arsenide, and the thermodynamic stability of the alloy with respect to the gallium arsenide.

5. LABORATORY DEVELOPMENT

In addition to the theoretical research described in the previous pages, we have designed a laboratory environment where the materials predicted to yield the best contacts can be tested. This has involved the ordering of a metallization system and the design and purchase of a clean room of the appropriate size and quality. Furthermore, recommendations were made to enhance the laboratory capability through the purchase of specific equipment items to test contacts and materials.

The metallization system purchased is a "desk top" sputter/evaporation system, specifically, the Balzers MED 010. This system has interchangeable heads which permit sputtering of refractory metals or compounds or physical evaporation of metals using the same basic apparatus. This saves the cost of purchasing and maintaining two separate systems. The system is compact and easy to operate. Pump down time is 10 minutes instead of one-half hour or more for larger systems. Use of this system will permit the sputtering of TiN or TiWN films for buffer layers and then by switching heads, the evaporation of Au, Ag, or other contact metals.

To prevent contamination of the specimens by airborne particles, we designed and purchased a clean room to house the test and fabrication equipment. The principal concern is chemical contamination which would produce anomalous results in calorimetry tests. In the future, it will be possible to construct high quality solar cells free from electrical faults caused by the inclusion of airborne dust particles.

The room has 218 ft² of usable floor space. Entry is facilitated by a gowning room covering 54 ft². Five individually operated HEPA filter units provide class 100 air for the clean room. With recirculation of the filtered air, we expect the air quality to be maintained at a level better than class 500. This means that at a height greater than 36 inches from the floor, there will be no more than 500 particles, 0.2 μm in diameter, per cubic meter. This room should be more than adequate for the laboratory needs.

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