(NASA-CR-195845) C.A.D. REPRESENTATION OF TERNARY AND QUATERNARY PHASE DIAGRAMS Final Technical Report (Michigan Technological Univ.) 17 p

N94-34170

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Michigan Technological University

NASA-CR-195845

C.A.D REPRESENTATION OF TERNARY AND QUATERNARY PHASE DIAGRAMS

Final Technical Report (Cooperative Agreement NCC3-183) *

This work is concerned with the utilization of C.A.D. solid-modeling software for the computer representation of three-dimensional phase diagrams. The work was undertaken in two parts.

First, the C.A.D. software (I-DEAS, by Structural Dynamics Research Corp.) was integrated with a variety of auxiliary Fortran 77 and I-DEAS language programs which were written specifically for the purpose of phase diagram representation. The capabilities of the resulting suite of software for three-dimensional phase diagram representation were developed and illustrated by the construction, display and manipulation of solid-model phase diagrams for a hypothetical quaternary eutectic system. The results of this work are discussed in some detail in the attached publication ("Solid-modeling: a C.A.D. Alternative for Three-dimensional Phase Diagram Representation'). Such a technique is of general applicability, having utility in both research and education.

Secondly, using the C.A.D. technique, data from the literature (gleaned from some 70 separate publications), which represent experimentally determined phase boundaries, were combined to form solid-model representations of the CMS_2-M_2S-S ternary space diagram and the CMS_2-CAS_2-M_2S-S quaternary liquidus projection (where C=CaO, M=MgO, A=Al_2O_3, and S=SiO_2). These diagrams were utilized in a concurrent study of solidification in the CMAS system; the solidification work was supported by the NASA Graduate Student Researchers Program (UMF) Grant #NGT-70514 (LeRC). Some examples of these diagrams and sections are given in Figures 1-3.

* The format of this final report was established in cooperation with the NASA technical officer associated with this project.

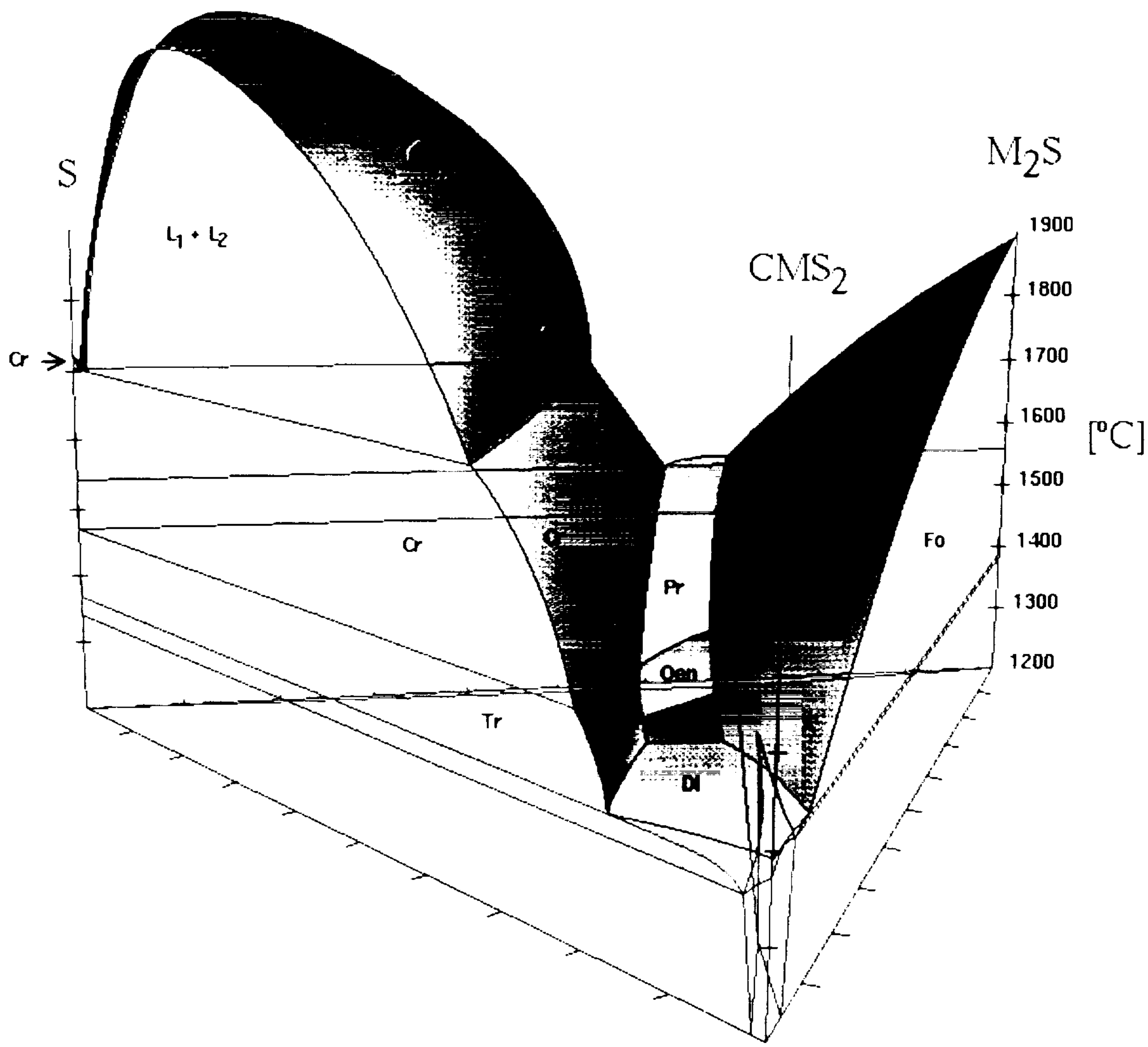

Figure 1. A shaded image display of the liquidus surface for the ternary subsystem CMS_2-M_2S-S.

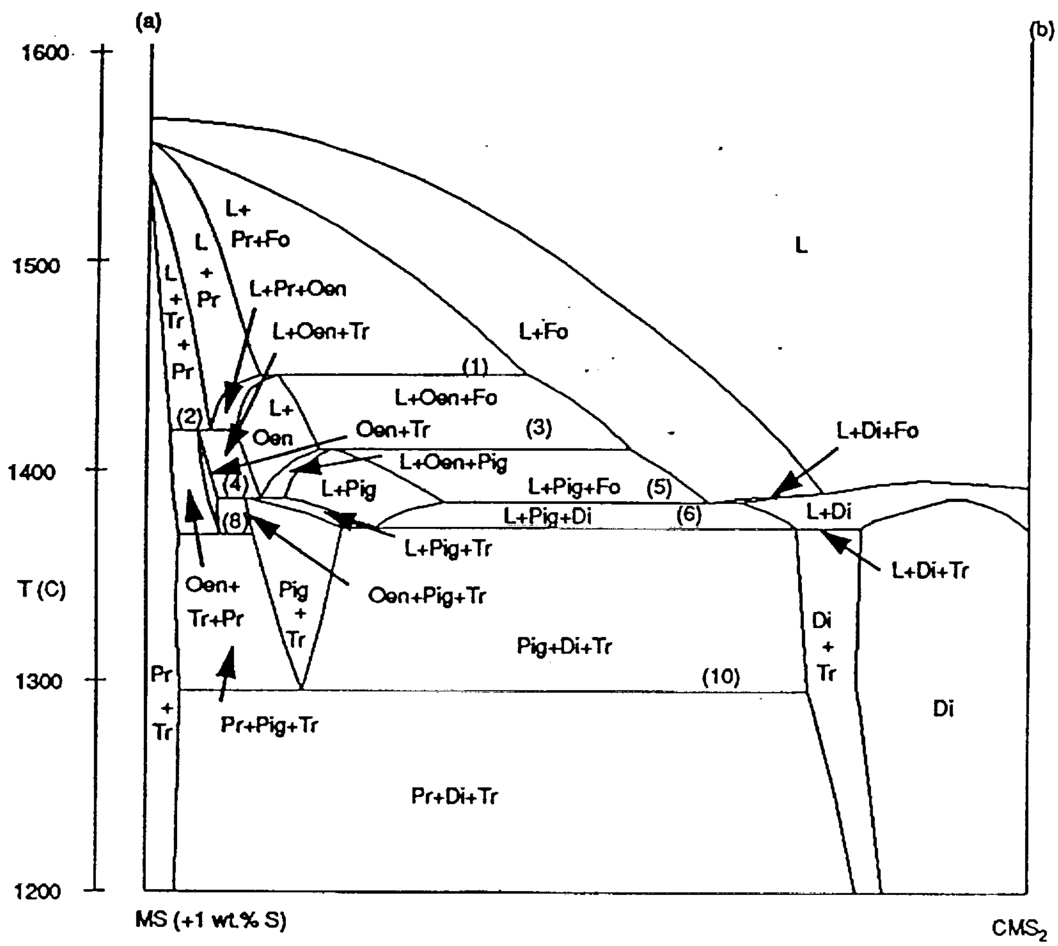

Figure 2. A vertical plane section taken from the silica-rich side of the MS-CMS_2 join in the CMS_2-M_2S-S space diagram (Figure 1).

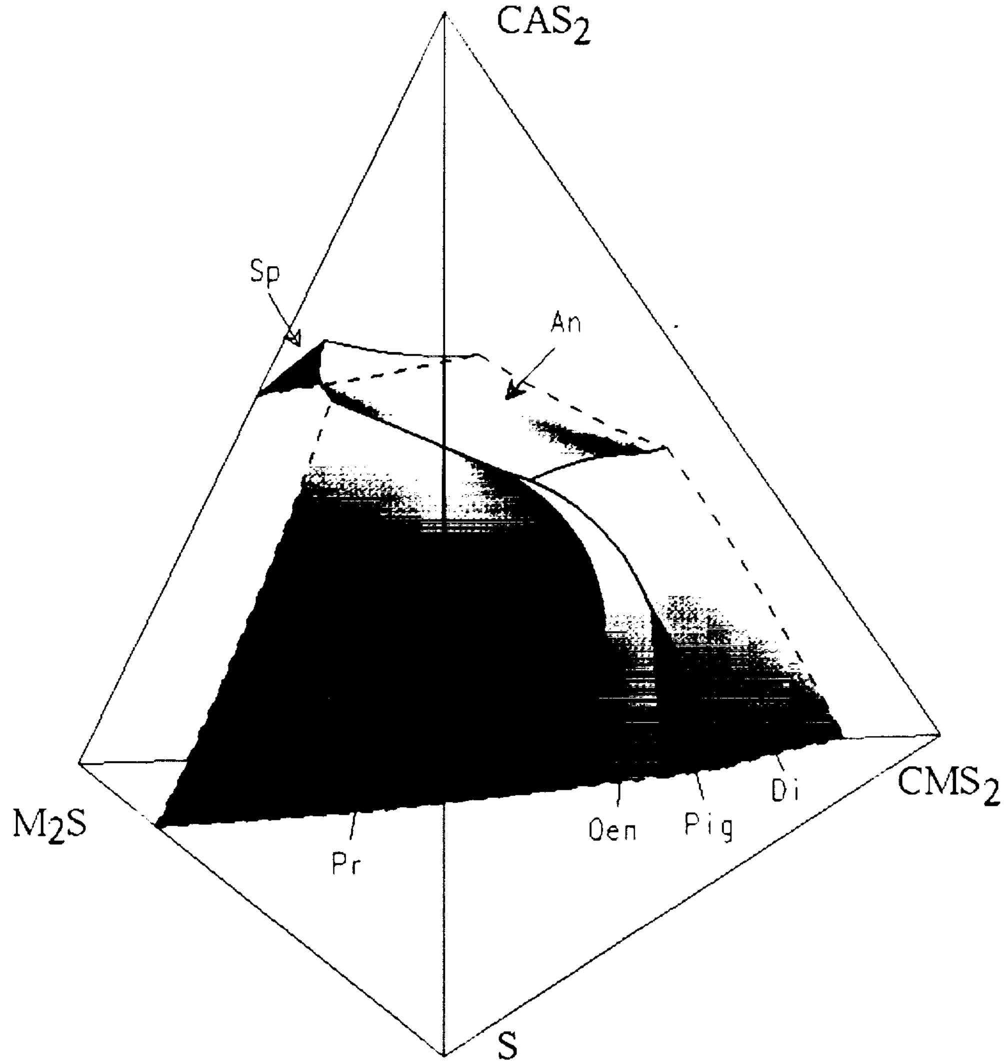

Figure 3. The Forsterite primary crystallization volume lies between the shaded surfaces (i.e., divariant boundaries, labeled according to the crystalline phase in mutual equilibrium with forsterite and liquid) and the M_2S apex of the liquidus projection.

SOLID-MODELING: A CAD ALTERNATIVE FOR THREE DIMENSIONAL PHASE DIAGRAM APPLICATIONS

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Abstract

Multicomponent materials are common in nearly all areas of materials science and technology, yet the use of phase diagrams to represent these complex systems is hampered by the requirement of three or more dimensions for explicit graphical representation. In the present work, the "solid-modeling" capabilities of a computer aided design (CAD) system have been applied to the representation of three-dimensional phase diagrams. Relevant phase diagrams for a hypothetical quaternary eutectic system were constructed and used to demonstrate the capabilities of the technique. These capabilities lead to relative ease of phase diagram construction and improved access to qualitative and quantitative information. Results of this work are contrasted and compared to previous efforts toward computer representation of phase diagrams. It is concluded that solid-modeling of three-dimensional phase diagrams can be used to advantage in both education and research.

Introduction

Equilibrium phase diagrams have proven to be indispensable tools for materials scientists and engineers. Simultaneously, work involving materials having several chemical components has been increasingly commonplace. However, in spite of an understanding of the topological rules for higher order phase diagrams (1,2,3,4), many difficulties inherent to the graphical representation of phase diagrams requiring more than two dimensions have greatly diminished their effective use.

The complexities introduced by the inclusion of a third dimension have prompted the development of several simplified alternative representations including, polythermal projections (3) and schematic representations of monovariant reaction paths (5). Such techniques are quite useful (as evidenced by their wide acceptance), however, they are simplifications and by their nature contain only a subset of the useful information available in the explicit three-dimensional representations. Thus, it has become necessary to develop means by which phase diagrams of dimension greater than two can be effectively utilized, thereby, extending the range of application of phase diagrams to more readily include chemically complex materials.

Toward this end, the application of the "solid-modeling" capabilities of a commercially available computer aided design (CAD) system to the representation of 3-D phase diagrams has been explored. It should be noted that the use of computers for phase diagram representation is not new, but dates back nearly 30 years. An excellent overview of such work is provided by Massalski (6). It is not the authors' intention to provide a review of the literature on this subject, although the results of the present work will be discussed partly in terms of these previous efforts.

CAD Representation of Phase Diagrams

Overall Approach

The objectives of this work were to develop efficient techniques for utilizing the capabilities of the CAD system and to demonstrate the usefulness of CAD "solid-modeling" for the representation of 3-D phase diagrams. Briefly, "solid-modeling", refers to the computer representation of "solid" objects as volumes enclosed by explicitly defined surfaces and is to be distinguished from earlier and simpler computer models known as "wireframes" wherein objects were defined only implicitly by frameworks of curves in three dimensions which outlined the edges of the objects.

To accomplish the above objectives, work consisted of the construction and manipulation of 3-D phase diagrams representing a hypothetical, completely symmetrical quaternary eutectic system. In order to develop a technique that would be generally applicable to real systems, input data used for the hypothetical system were chosen to be similar, both in kind and amount, to data which are typically available in the literature.

The CAD System

The CAD system used in this work consisted of a CAD software package known as I-DEAS and a Sun 4 Engineering Workstation. I-DEAS (Integrated Design Engineering Analysis Software) was created by Structural Dynamics Research Corporation and the version used, Level 4.0, was released in 1988. I-DEAS was chosen because of its solid modeling capabilities and wide availability.

The Sun workstation (a.k.a. Sparc) is similar in configuration to a personal computer consisting of a central processor, keyboard, color graphics monitor, external hard drive, and a conventional "mouse". The workstation is comparable in size to a personal computer, sells for approximately twice the price of a good PC, but has tremendously greater capabilities.

Phase Diagram Construction

Researchers who would utilize 3-D phase diagrams must begin with "construction" of the diagrams. Published phase diagram data for multicomponent systems are typically hierarchical, that is, binary subsystems are the most completely and reliably described with the availability and certainty of the data progressively decreasing with each additional chemical component. In keeping with this trend, binary subsystems, for the present work, were assumed to be completely described. Data for the ternary subsystems consisted of the information typically available from two dimensional polythermal liquidus projections supplemented by minimal subsolidus information. Finally, data for the interior of the quaternary system consisted only of points along the monovariant reaction paths.

The procedure used in this work was designed to take advantage of the more completely determined low-order systems. The binary subsystems were constructed first. Data, representing points along phase boundaries, for the binary eutectic system "A-B" were entered and displayed in the binary composition-temperature plane. The points were spline fitted to form curves depicting phase boundaries (Figure 1). It should be noted that the display of input data points can be suppressed so as to provide uncluttered images; this will be the case for all subsequent figures. The data points can be easily redisplayed however, giving users a clear knowledge of how precisely defined a given phase boundary might be, or conversely, to what extent a particular boundary is the result of approximation. It is also of interest to note that the curves and surfaces generated by the CAD system are represented internally as non-uniform rational B-splines (NURBs), a highly sophisticated representation which allows complex geometries to be modeled without introducing unwanted inflection points.

The binary subsystems "A-C" and "B-C" were created in a like manner, reoriented in space, and subsequently combined to define the sides of the "A-B-C" ternary space model (Figure 2). In this way, the relatively more complete information for the binary subsystems was used to aid in the construction of the ternary diagrams. Coordinates of points along monovariant paths within the space model were entered and curves were fitted to these points, thus completing the wireframe representation of the ternary phase diagram (Figure 3).

The ternary space model was subsequently completed by utilizing a variety of solid-modeling techniques available with the I-DEAS software to generate surfaces "supported", as it were, by the curves of the wireframe model. The construction techniques used for any given surface were dependent upon the available data. Unfortunately, some surfaces (e.g., solvus surfaces), where only a few internal data points were used to supplement the wireframe representation of the surface edges, had to be generated by using least

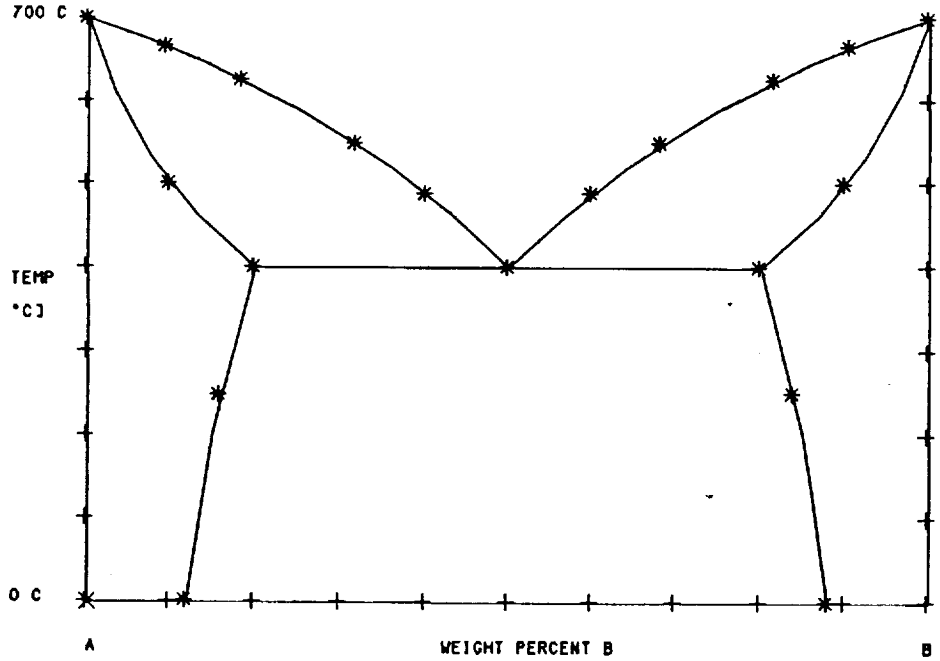

Figure 1 - Input points and interpolated phase boundaries for the hypothetical binary eutectic system "A-B" (from laser printer).

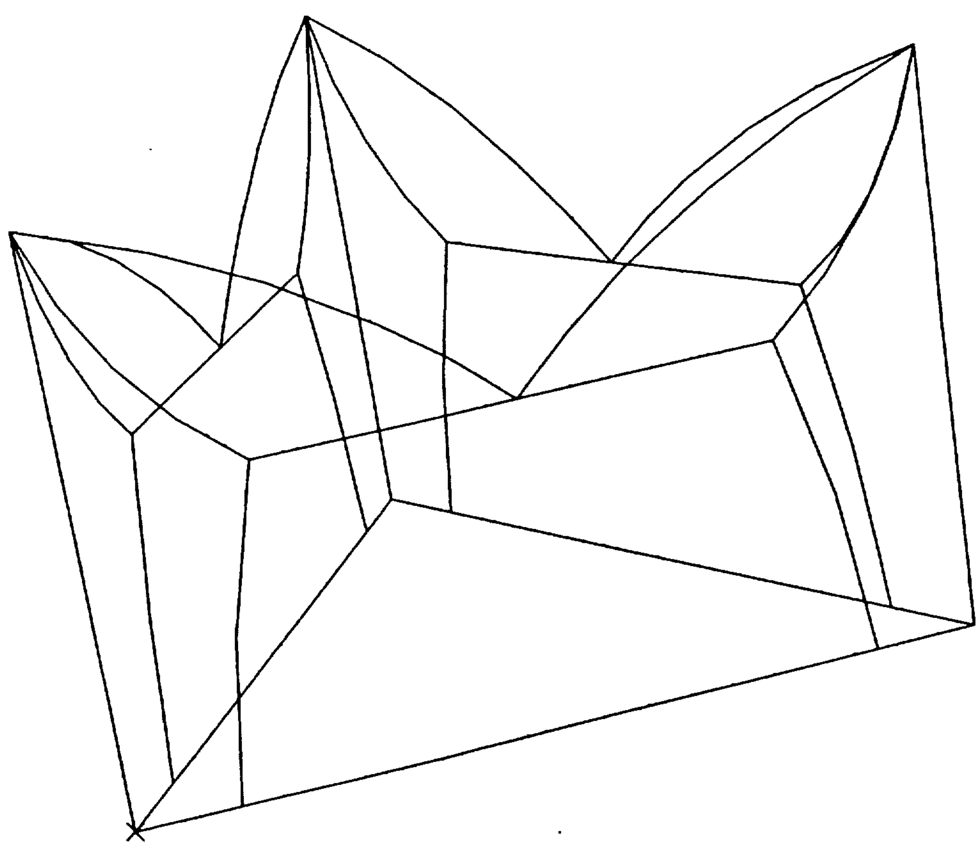

Figure 2. Diagrams for the binary subsystems "A-B", "A-C" and "B-C" are combined as a first step in constructing the "A-B-C" ternary space model (from laser printer).

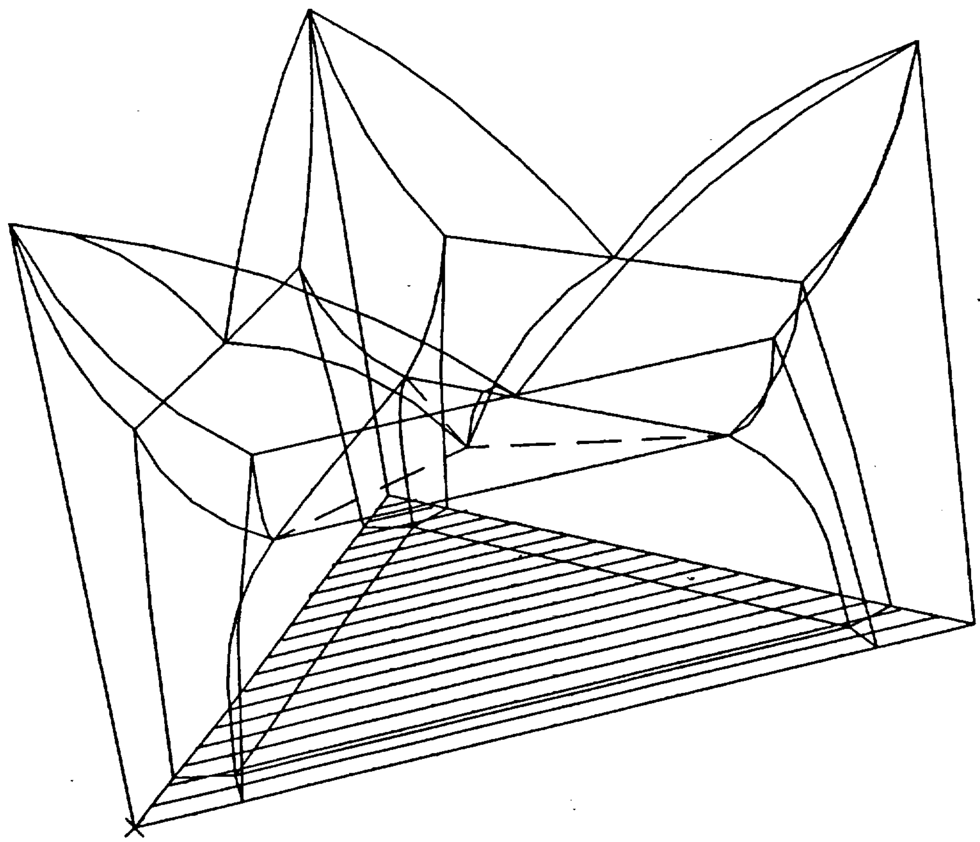

Figure 3 - A completed "wireframe" representation of the hypothetical ternary "A-B-C" (from laser printer).

squares or interpolation fits; such surfaces are obviously only somewhat loose approximations. In such cases, it is possible to place limitations on possible geometrical configurations by making use of the rules that govern the topology of phase diagrams of the appropriate order. CAD system features such as instantaneous display of generated geometry and the ability to view the solid-model from any spatial location greatly facilitate user interaction to verify the topological legitimacy of the constructions in question.

Utilizing the various surface generation techniques, each phase region was constructed and stored as a separate closed "solid-object" having associated with it an appropriate name (e.g. alpha + liquid, for the corresponding phase field). The complete phase diagram was assembled defining a "system" composed of the individual phase regions (each having associated with it a spatial orientation). Figure 4, shows a "system" composed of the phase regions for the "A-B-C" ternary diagram. However, in this figure the system was defined to include translation vectors for each phase region, thus moving the regions apart to create the "exploded" configuration shown. This construction procedure was repeated for the remaining ternary subsystems.

As a first step in creating an isothermal quaternary diagram, isothermal cross-sections were taken at the desired temperature through each of the four ternary space models (Figure 5a). These cross-sections were reoriented and combined to form the faces of the isothermal, quaternary tetrahedron, once again, using the more fully defined low-order systems to aid in construction of the diagram for the high-order system (Figure 5b).

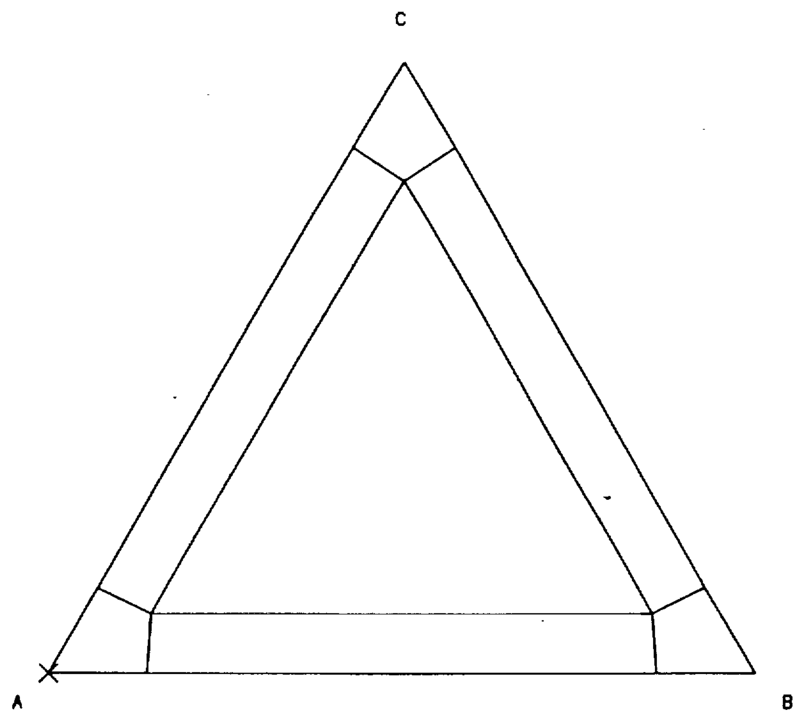

Figure 5a - A subsolidus isothermal cross-section through the "A-B-C" phase diagram (from laser printer).

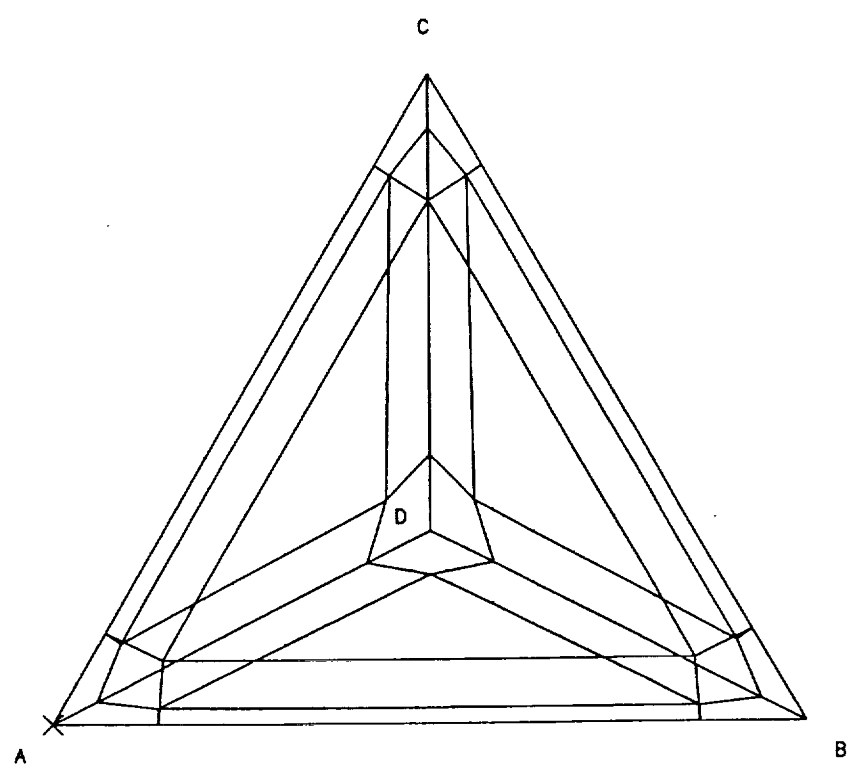

Figure 5b - Isotherms from the ternary subsystems are combined to begin construction of a quaternary isothermal diagram.

Phase Diagram Display

Given the importance of qualitative information which can be ascertained by visual inspection of phase diagrams, it is critical to represent 3-D phase diagrams in such a way as to facilitate visual comprehension. CAD solid-modeling provides many sophisticated features which can be used to clarify the display of complex images.

Displays of phase diagrams with shaded surfaces can be created which include silhouettes, shadows and translucent surfaces. The appearance of shaded images can be tailored by adjusting display attributes, which include degree of transparency (0% - 100%), color, diffuse reflectivity, glossiness and radiance, individually, for each surface or solid object as well as controlling the types and positions of individual light sources. Furthermore, line drawings, such as coordinate systems, series of stored tie-lines, or planar cross-sections can be superimposed onto the shaded images to highlight various features or add clarity. The use of shaded images are illustrated in the display of an "exploded" ternary (Figure 6), shown as a line drawing earlier in Figure 4, and a subsolidus quaternary isotherm (Figure 7). Unfortunately, much of the clarity and contrast is lost when the images are transposed to black and white.

"Dynamic viewing" of the solid-model (without shaded images) allows the observer to change point of view in a continuous, interactive manner; the view of the model can be rotated (in 3-D, about any combination of axes), zoomed, or translated, all in real time, simply by movement of the "mouse" about its pad. These same view changes can be accomplished discontinuously with greater precision by entering the view change from the keyboard (e.g., rotation about a specified axis: $+30^\circ$). These features can be used alone, or in conjunction with other features, such as, shaded image displays. For example, dynamic viewing could be used to choose a desired point of view, a shaded image could be generated having that view and a coordinate system could be superimposed on the shaded image. To further enhance visual comprehension, the viewing screen can be subdivided and the image in each "viewport" can be individually tailored using the features described above so that several different displays of a phase diagram can be viewed simultaneously.

Extraction of Information

Many types of valuable information can, in theory, be extracted from 3-D phase diagrams, however, gaining access to this information has traditionally been a difficult task. The use of CAD solid-models for phase diagram representation makes the determination of composition and/or temperature for a point on a phase boundary a simple task. The point in question can be selected in a variety of ways and since all boundaries (surfaces and curves) have mathematical representations, the coordinates of the point can be quickly determined by the computer and displayed on the viewing screen.

Phase fractions, for given bulk composition and temperature, can be calculated if the compositions of the phases in mutual equilibrium are known. It is therefore a simple matter in monovariant phase regions, which are invariant for fixed temperature conditions, to determine the compositions of the relevant phases from the diagram and, thus, to calculate the phase fractions. A short program was written, using Ideal, to automate the process of phase composition determination and phase fraction calculation. Of course it is a simple process, given the appropriate

Figure 6 - A shaded image display of an "exploded" ternary diagram as photographed in black and white from the computer monitor.

physical constants for the relevant phases, for the computer to convert between mole fractions, weight fractions and volume fractions. Furthermore, the ability to calculate phase fractions for monovariant regions quickly and repeatedly at desired intervals over a range of temperatures can be used to determine the nature of a monovariant reaction (e.g., liquid + alpha → beta + gamma vs. liquid → alpha + beta + gamma) for a given bulk composition, using Hillert's criterion (7). However, by using a technique that actually determines phase fractions, the difficult graphical constructions necessary for such an evaluation using pencil and paper would be avoided.

Determination of phase compositions for equilibrium phase associations which are monovariant or divariant at a fixed temperature is a more difficult task. In this case, if tie-lines or tie-triangles are

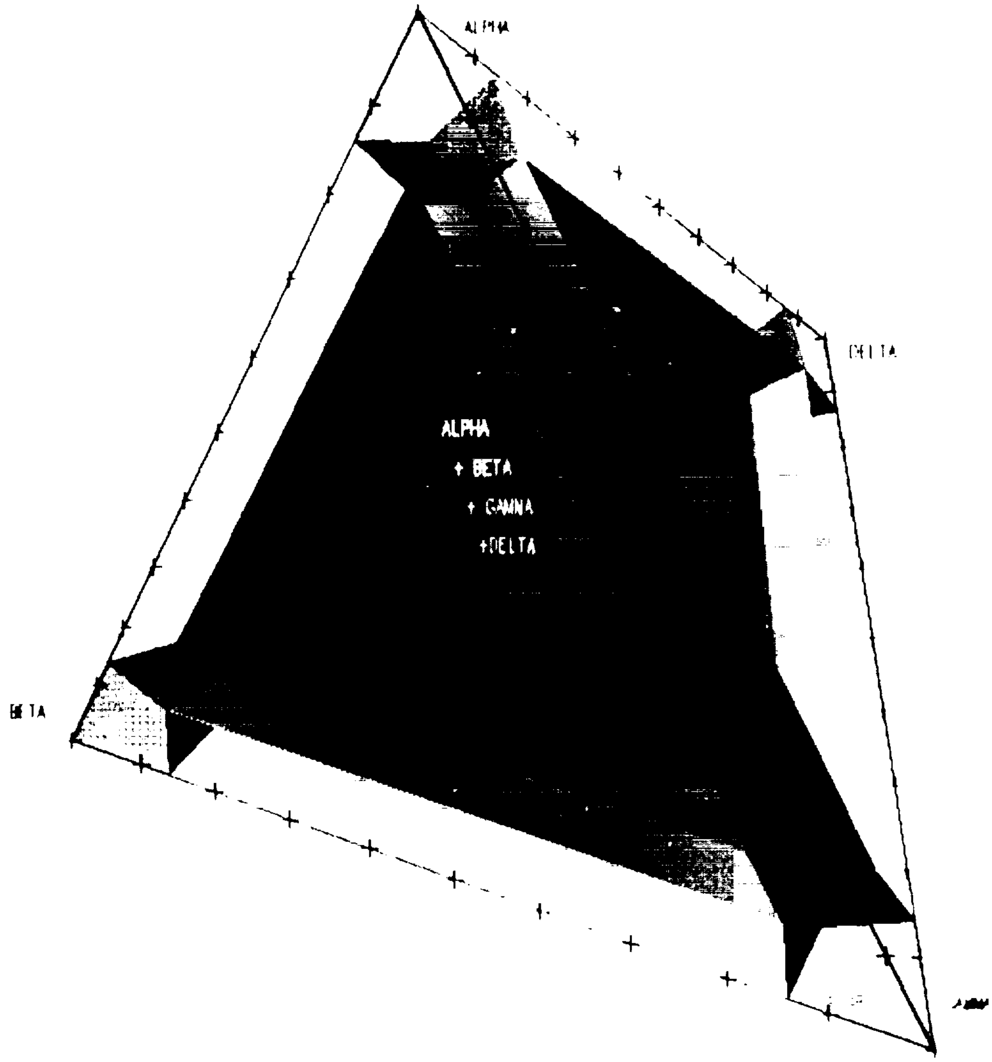

Figure 7 - A shaded image display of a quaternary isothermal diagram (see Figure 5b) using translucent surfaces (photograph).

available from the literature, they can be stored as line drawings and superimposed on the phase diagram to aid in approximation of the compositions of phases in equilibrium. Once again, this information can be used to calculate phase fractions.

The use of solid-models, having explicitly defined surfaces is also helpful for the extraction of geometrical information, for example, planar sections through 3-D diagrams. In this case the user merely orients the "cutting plane" using a wide variety of available techniques; the rest is automatic. Figure 8a, shows an isothermal planar section, taken through the "A-B-C"

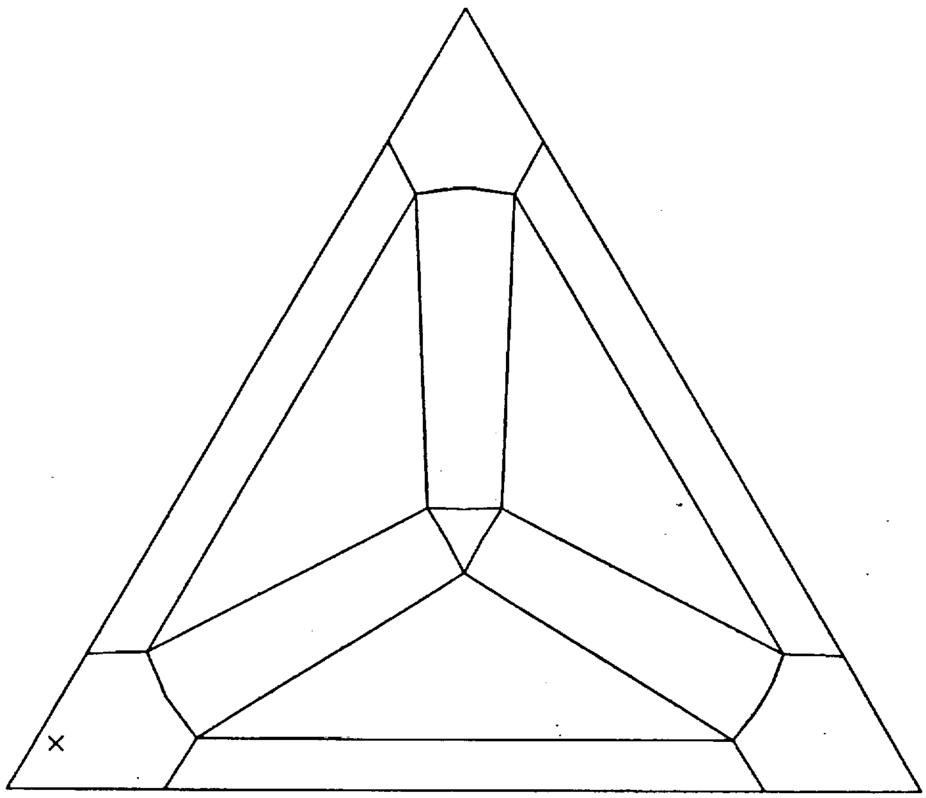

Figure 8a - An isothermal cross-section through the ternary system "A-B-C" as produced by the sectioning process (from laser printer).

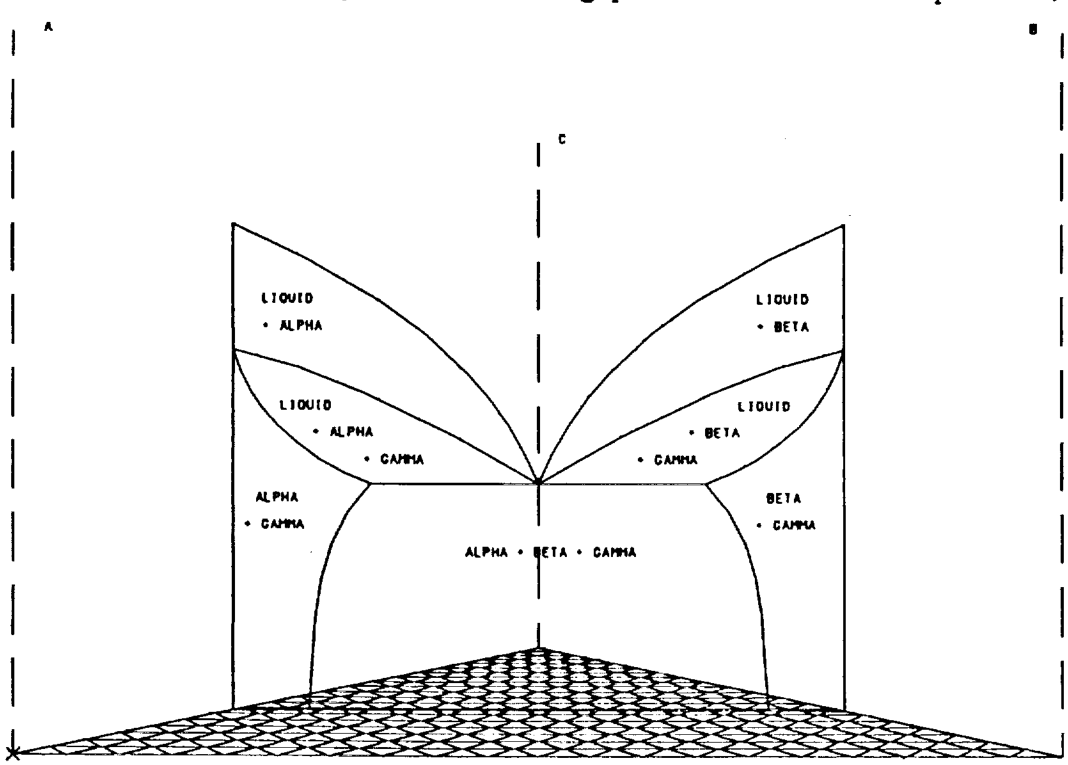

Figure 8b - An isopleth through the system "A-B-C" enhanced by the addition of labels and a coordinate system (from laser printer).

ternary diagram at a temperature less than the binary eutectic and greater than the ternary eutectic invariant. The section in this figure is presented exactly as generated by the cutting operations. Figure 8b, is a vertical section, taken through the same diagram at a constant fraction of component "C" (i.e., an isopleth) and passing through the ternary eutectic point. This diagram has been enhanced by adding labels and superimposing the ternary coordinate system.

Discussion

Various computer methods for the representation of phase diagrams have been proposed and used. Much of the work in this area has been aimed at computer calculation of phase diagrams using thermodynamic models. To the authors' knowledge, no programs are available which have been intended primarily to assist researchers working with multicomponent materials in the efficient construction (from experimentally determined phase boundaries) and use of 3-D phase diagrams. However, a small number of computer programs have been written which are dedicated to various aspects of phase diagram applications, which could conceivably be put to use in a manner similar to that discussed in the present work. Most prominent among this list is a large scale computer based phase diagram project underway at the NIST (8). However, to the author's knowledge these programs are still being developed and are not generally available for such a task. Of the phase diagram programs currently in use, one of the most widely cited is that of Schultz and Chang (9). However, the availability of CAD systems capable of solid-modeling have provided researchers with powerful new tools; tremendous resources have been devoted to the development of these systems, thus providing many highly sophisticated features which offer several advantages to the user.

There are many powerful features which are largely unique to CAD systems. A partial list of such features available with the CAD system used in this work (many of which have been discussed above) would include: dynamic viewing, translucent shaded surfaces, the automated capability of creating and joining planar cross-sections, the capability to utilize non-uniformly spaced input data, faceted representations of surfaces which can be non-uniformly spaced (allowing finer facets in more complex areas), the use of nonuniform rational B-spline curves and surfaces, and the immediate display of data entered and geometry generated. Furthermore, CAD programs are high level, menu-driven programs which do not require the user to possess advanced programming skills. (It should not be surprising that a CAD system with solid-modeling capabilities provides many features which facilitate the use of 3-D phase diagrams; such systems were specifically designed to conveniently and effectively assemble, display, and manipulate three dimensional geometry.) Moreover, CAD systems are widely available in research laboratories, whether in educational institutions, government labs, or private industry. Thus, in many cases, no new hardware or software acquisitions are necessary.

In spite of the merits of CAD systems for phase diagram applications, very few researchers have attempted to utilize CAD systems for this work. To the authors' knowledge, previous work using CAD systems (e.g., Roeder (10)) was limited largely or entirely to wireframe representations. Unfortunately, without solid-modeling, many of the advantages of CAD representations are sacrificed. The lost capabilities include: shaded surface displays, efficient and self-consistent generation of planar sections through diagrams, and self-consistent determination of composition-temperature coordinates for phase boundary surfaces.

Conclusions

The CAD solid-modeling technique described in this paper clearly demonstrates potential benefits for phase diagram applications. However, CAD systems are obviously not capable of direct application to phase diagrams having four or more dimensions. Therefore, explicit representation of phase diagrams are confined to systems of four or fewer chemical components.

Nonetheless, it is envisioned that CAD solid-model representations of 3-D phase diagrams can be used to advantage both in education and research. In education, the versatile and vivid displays of phase diagrams made possible by this technique could be used with great advantage to illustrate the topologies of ternary and/or quaternary phase diagrams; a traditionally difficult area of instruction. Furthermore, researchers whose work involves three or four component materials could apply CAD solid-modeling to aid in the effective use of relevant phase diagrams.

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