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DIPHASIC DOMAINS APPROACH METHOD (DDAM)
Binary and ternary phase diagrams plotting

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If someone wants to plot an isobaric temperature-composition binary or an isobarothermal section of a ternary equilibria phase diagram he only needs to plot the limits of diphasic domains, it automatically gives the limits of the monophasic and triphasic fields. In such diagrams each diphasic domain is defined by two lines joining all the extremities of the tie-lines of the domain and limited by the first and the last one. These tie-lines are segments whose the extremities are in the plane of the diagram and can easily be determined by equilibria calculation codes. Then binary or ternary phase diagrams can be plotted only using conodes of the diphasic fields and the method used to determine the diphasic domains becomes the main point in binary and ternary phase diagrams plotting. A meshing of the surface of the diagram is certainly not the best way to obtain a rapid result. We propose an approach which consists to follow the curvature of the diphasic domains limits, the 'Diphasic Domains Approach Method, DDAM', which allows a rapid and robust determination of binary and ternary diagrams.

Keywords: *Calphad, DDAM, diphasic domains, diphasic domains approach method, phase diagram, plot, thermodynamics*

Introduction

The ultimate step in the Calphad method (computer coupling of phase diagrams and thermodynamics) [1] is the graphical representation of the results, and in first the plot of binary and ternary calculated equilibrium phase diagrams. Each one among us was confronted with this problem and it should well be acknowledged there is not for the moment an entirely automatic and satisfactory procedure which starting from the file of the optimized parameters of the various phases energy potentials gives the corresponding equilibrium phase diagram without any ungraceful kink or without the intervention of the user. The subject seems to be ridiculous but many are those who tried to approach it without obtaining a total success.

At the basis of our work there is an observation: if someone wants to plot an isobaric temperature-composition binary or an isobarothermal section of a ternary equilibria phase diagram he only needs to plot the diphasic domains. It automatically gives the limits of the monophasic and triphasic fields.

In such diagrams each diphasic domain is defined by two lines joining all the extremities of the tie-lines of the domain, also called conodes, and limited by the first and the last one. These tie-lines are segments whose the extremities give the compositions of the two phases in equilibrium in the diphasic domain. They are in the plane of the diagram and can easily be determined by equilibria calculation codes.

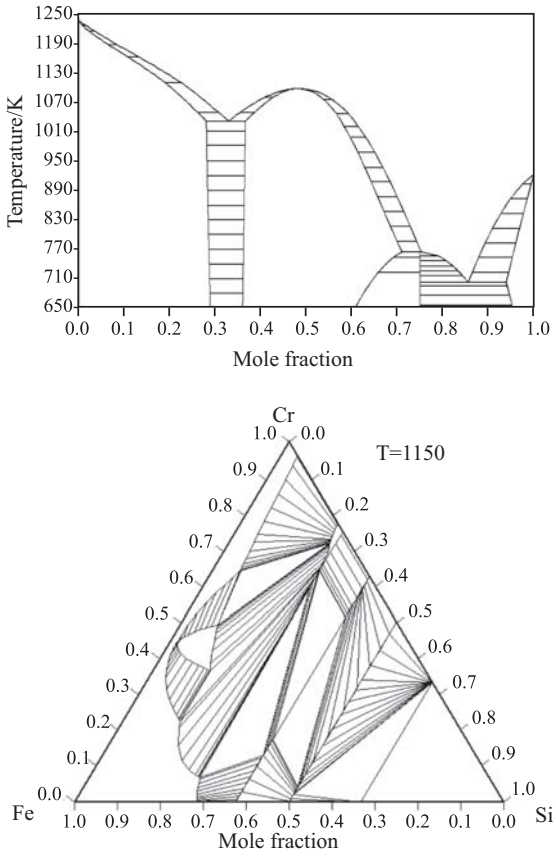

Fig. 1 Binary and ternary diagrams plotted from the conodes of the diphasic domains

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Then binary or ternary phase diagrams can be plotted only using conodes of the diphasic fields (Fig. 1) and the method used to determine the diphasic domains becomes the main point in binary and ternary phase diagrams plotting.

The first idea coming in mind to plot such diagrams is to do a fine meshing of the whole surface. But every body can rapidly see that it is not the best method because it needs many calculation steps and then it is time consuming, more limits of phases are given in this case by calculations in the vicinity, zone in which equilibria are the most difficult to determine. We propose a curve follow approach adapted to each case which allows a rapid and robust determination of diphasic fields: the diphasic domains approach method.

Binary diagram: the median method

The first conode of a diphasic domain is something easy to find scanning the limits of the diagram. Here on Fig. 2 the first conode is a single point, it is the HCP/liquid transition of cadmium. Starting from that point n° 1 a step delta in temperature and composition inside the diagram is carried out to obtain the second conode. An analysis on the circumference of the circle centred on that first point with a delta radius allows to rapidly find with three calculations only, the conode n° 2.

From these two conodes the segment with a delta length going from the middle of the last conode in the direction given by the line linking the middles of the two last conodes allows to determine the composition and temperature of the next calculation which will give a third conode with optimal conditions. The process is then continued by using the two last conodes until the limits of the diagram. The step delta should not inevitably be very small to lead to a sufficient precision of the diagram it depends on the form of the

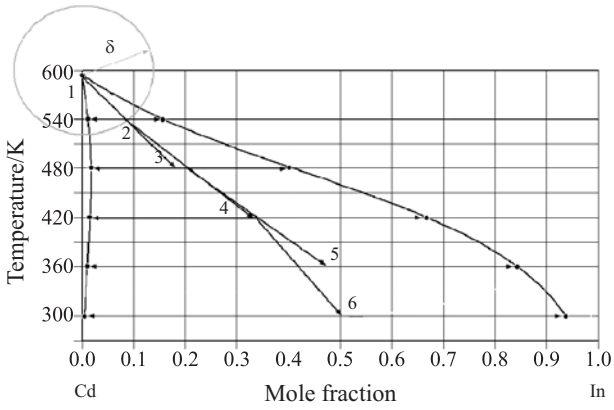


Fig. 2 Follow-up of the curve of the limits of a diphasic domain in a binary system

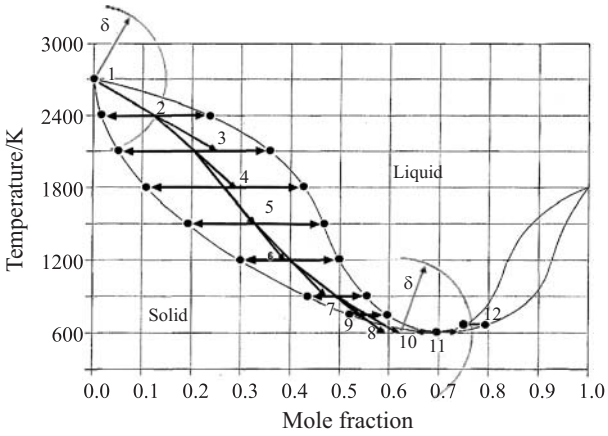


Fig. 3 Follow-up of a diphasic field presenting an optimum

limits of phases and the method of interpolation used between the calculated points. It is also possible to accelerate or decelerate the procedure while acting on the value of delta according to the monotony of the curve which can be evaluated on a conode by the comparison of the distance which separates the middle of the conode and the total composition used for the calculation of this conode to the length of the conode. The example of Fig. 2 shows that generally less than ten conodes are enough to determine a two-phase field very precisely when this one does not have extravagance.

Some complications can appear, it is the case when the two-phase field becomes very narrow and/or presents a passage by an optimum. Figure 3 illustrates this case and the method of follow-up proposed.

The beginning of the procedure is the same one as previously described, which allows the determination of the 7 first conodes. Then the calculation of the eighth conode, made starting from the point of total composition and temperature given by the segment which passes by the middles of the conodes 6 and 7 and with a length delta, indicates the passage in a single-phase field. At this time there the step delta is divided by two, which allows the calculation of the conode n° 9. The next point of calculation, with a step delta/2, gives a single-phase domain. Let us admit that the criterion of stop of reduction in the step is reached, then to continue it will again be necessary to apply the starting procedure that was applied on point 1 to find the conode 2. We apply this procedure to point n°10, with the initial step delta, which makes it possible to find the conode n° 12 quickly. To define the point n°11 it is enough to remember the empirical rule of Konovalov which says this: 'In a binary diagram, at constant *P*, *T* takes extreme values for a two-phase equilibrium if the two phases reach the same composition'.

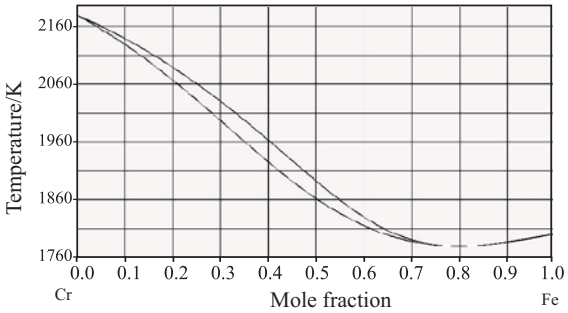


Fig. 4 Diphasic field BCC/liquid in Cr–Fe

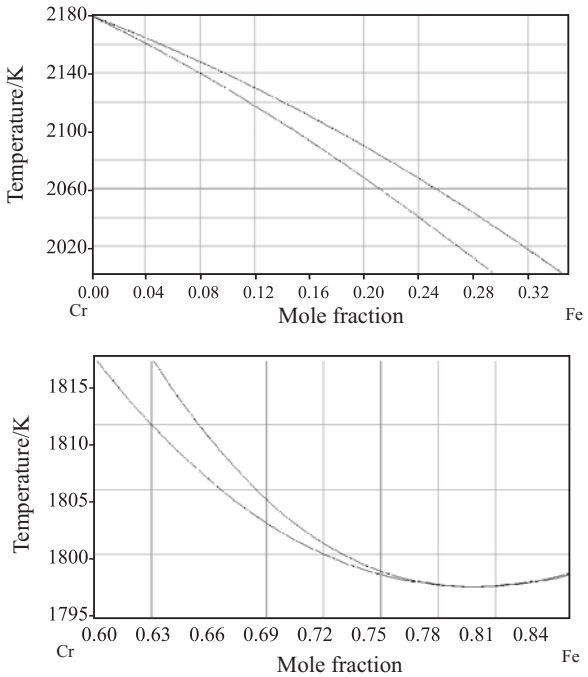


Fig. 5 Diphasic domain BCC/liquid in Cr–Fe: details

It is thus enough to introduce into the procedure of interpolation, which starting from the ends of the calculated conodes makes it possible to trace the limits of the diphasic domain, this singular point for which the tangents with the curves must be confused and horizontal.

This method of the median gives very satisfactory results even in the most difficult cases as shown on Figs 4 and 5.

Ternary diagram: the mediatrice method

The procedure developed for the follow-up of diphasic domains in the ternary systems is quite different. We will use in that case the mediatrice of the conode to progress step by step in the domains. It is thus necessary from one of the tops to scan a bordering binary until finding a first conode. Then a step in composition is made in the direction given by the mediatrice of this first conode to determine the following conode and so on until leaving the two-phase field. If the exit is carried out on a single-phase current it is necessary to reiterate on the bordering binary starting from the point where it had been left. If the exit of the diphasic is done on a triphasic domain it is necessary to con-

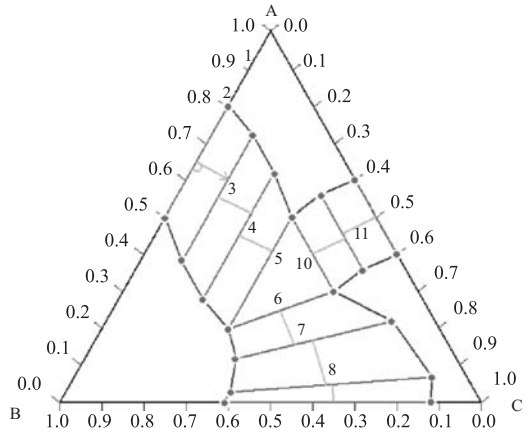
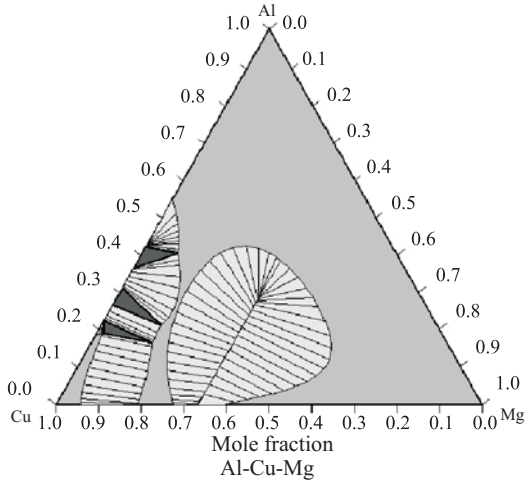


Fig. 6 Follow-up of the curve of the limits of binary domains in a ternary



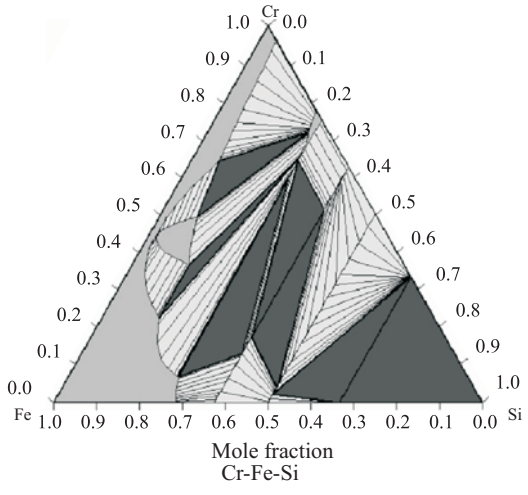


Fig. 7 Examples of calculated ternary diagrams

tinue the analysis by taking like first conode each of the two other sides of that triphasic. Figure 6 illustrates this procedure.

This method of the mediatrice gives excellent results as Fig. 7 shows it.

'DiagPlot'

This effective and flexible application was developed to plot the equilibrium phase diagrams of binary and ternary systems calculated using the procedures described previously. Easy to use, 'DiagPlot' allows a total control of the edition of the diagrams. This application is an integral part of 'ThermoSuite' [2], a software whose objective is to allow the chemists and the materials engineers to have a thermodynamic approach of their complex problems.

The points, lines and surfaces, calculated with any software of determination of equilibrium state must be structured under a very convivial ASCII format. Hereafter Fig. 8 shows us an example of a binary diagram with only three points calculated by field.

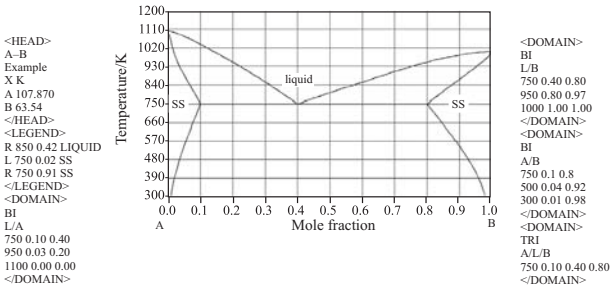


Fig. 8 Data file and corresponding plot

Conclusions

These two procedures of follow-up of the diphasic fields are simple to implement, effective and robust. We integrated them in our software package of automatic plot of binary and ternary phase diagrams and the results obtained are more than satisfactory as well on the speed of calculation as precision of the results.

Acknowledgements

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References

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2 Calphad, 26 (2002) 167.

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