Calculating Phase Diagrams Using *PANDAT* and PanEngine

S.-L. Chen, F. Zhang, S. Daniel, F.-Y. Xie, X.-Y. Yan, Y.A. Chang, R. Schmid-Fetzer, and W.A. Oates

Author's Note: Trial versions of *PANDAT* and PanEngine may be downloaded at www.computherm.com.

Editor's Note: A related article, "Our Experience in Teaching Thermodynamics at the University of Wisconsin, Madison," by Y. Austin Chang and W.A. Oates, is available on-line only at www.tms.org/pubs/journals/JOM/0312/Chang/Chang-0312.html.

Knowledge of phase equilibria or phase diagrams and thermodynamic properties is important in alloy design and materials-processing simulation. In principle, stable phase equilibrium is uniquely determined by the thermodynamic properties of the system, such as the Gibbs energy functions of the phases. PANDAT*, a new computer software package for multicomponent phase-diagram calculation, was developed under the guidance of this principle.*

INTRODUCTION

Knowledge of phase equilibria and thermodynamic properties is necessary for alloy design and materials-processing simulation. Because most alloy materials have from five to 15 components, a tool is needed to provide information regarding phase equilibria and thermodynamic properties for multicomponent systems. Such a tool requires a thermodynamic database and calculation software. (A brief history of phase diagram calculation can be found in the sidebar.)

The thermodynamic database is a collection of thermodynamic properties of the phases in the multicomponent alloy system. Due to the combinatorial complexity of a multicomponent system, such a collection generally covers only the properties for the pure components, the constituent binaries, and key ternaries. Little information is included for quaternary or higher order systems. The second part of the tool is the computer software that uses the information in the thermodynamic databases to calculate the phase equilibria or diagrams and the thermodynamic properties.

Unfortunately, however, the available software sometimes is unable to handle phases that have multiple minima in the Gibbs energy function and therefore fails to calculate the correct stable phase diagram. In these cases, it is necessary for the user to know, a priori, the stable phase diagram that he/she wishes to calculate so appropriate initial values may be given to guide the software. Examples of published calculated binary phase diagrams that contain metastable phase boundaries can be found in Reference 16.

This inability to find the stable equilibrium requires some special skills on the part of the user: before the calculation is made, the user must ensure that the calculated phase diagram is the stable one with regard to the thermodynamic parameters of phases and the system constraints imposed. For complex, multicomponent systems it is almost impossible for a user to have either the prior knowledge or the necessary skills, and thus, it is easy to obtain an incorrect phase diagram. To resolve those problems, the authors developed *PANDAT* software for the calculation of phase diagrams and thermodynamic properties.

PANDAT

PANDAT is designed to calculate the most stable phase equilibrium automatically. It uses a global minimization algorithm based on the mathematical and thermodynamic properties between the Gibbs energy function and the stable phase equilibrium. C++ was chosen as the language and Microsoft Windows© was chosen as the initial platform for *PANDAT*'s development. The software

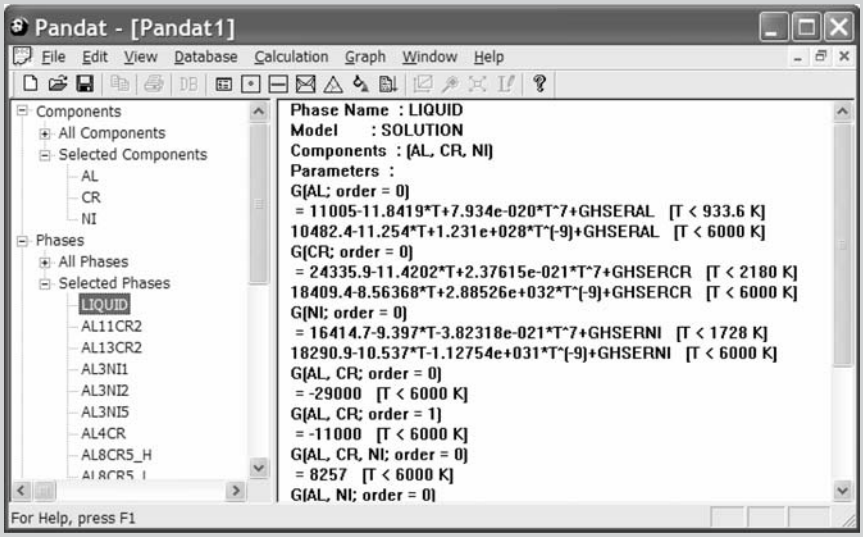

Figure 1. The *PANDAT* main Windows interface.