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DEVELOPMENT OF ICALPHAD SOFTWARE FOR PHASE DIAGRAM CALCULATION AND INTELLIGENT THERMODYNAMIC OPTIMIZATION

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Abstract
This paper presents the ICALPHAD software, which enables the calculation of phase diagrams and thermodynamic properties for various material systems. The software integrates a new optimization algorithm based on multi-objective optimization to efficiently handle incomplete or missing experimental data. Key features include modules for binary and ternary phase diagrams, thermodynamic property calculations (e.g., Gibbs energy, enthalpy, heat capacity), and the ability to model external conditions such as magnetic fields. These developments demonstrate the potential of the software as an intelligent platform for phase diagram calculation and thermodynamic optimization in computational materials science.

***Keywords**: ICALPHAD, optimization, phase diagrams, thermodynamics, multi-objective optimization.*

1. INTRODUCTION

Accurate calculation of phase diagrams and thermodynamic properties is essential for materials design and process optimization. The CALPHAD method provides a well-established framework for such calculations, but existing tools often require complete datasets and involve complex manual optimization steps [1]. To address these limitations, the ICALPHAD software has been developed as a modular and extensible platform. It integrates binary and ternary phase diagram modules, thermodynamic property calculations, and external field modeling. A key feature is an intelligent optimization framework based on multi-objective methods, which improves efficiency and reliability when experimental data are incomplete [2]. The software is designed with an engineering-oriented graphical interface, supporting streamlined data input, automated parameter handling, and real-time visualization. This makes ICALPHAD suitable for both research and industrial applications where accuracy, robustness, and usability are critical.

2. SOFTWARE DEVELOPMENT

ICALPHAD has been developed as a modular and extensible software platform for the calculation of phase diagrams and thermodynamic properties. Its design philosophy emphasizes flexibility,

reusability, and scalability, making it suitable for both academic research and industrial applications. The software consists of several functional modules that can operate independently or in combination, ensuring that users can tailor calculations according to their needs.

2.1 Binary Phase Diagrams

The binary phase diagram module enables the calculation of multiple binary alloy systems, such as Ag-Pb, Al-Ta, Cu-Mg, and Fe-Ni. Each binary system can be independently loaded through database files, and the software supports visualization of equilibrium phase boundaries, liquidus and solidus curves, as well as metastable extensions. Special attention has been given to accuracy and flexibility, allowing researchers to dynamically adjust composition and temperature ranges.

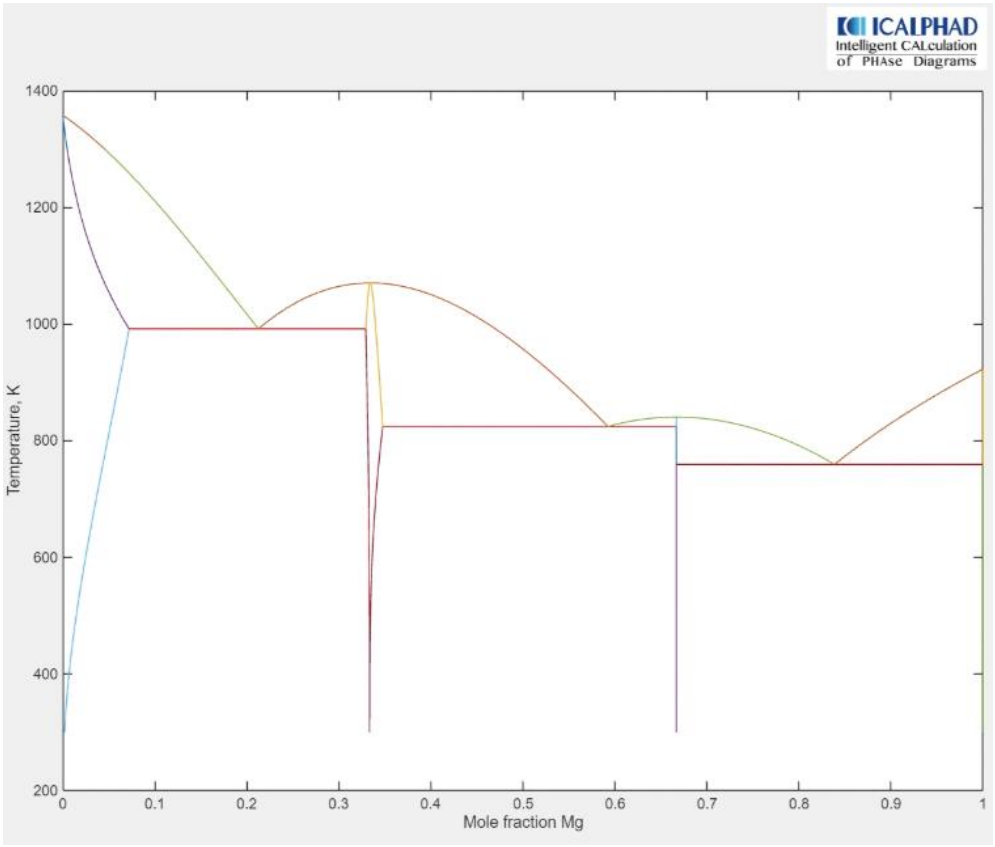

Figure 1. Cu-Mg binary phase diagram calculated by using ICALPHAD software

2.2 Ternary Phase Diagrams

For ternary systems, ICALPHAD provides dedicated modules for both isothermal sections and vertical sections. For example, in the Fe-Mo-Zr system, users can generate phase diagrams across a range of fixed temperatures (isothermal sections) or along specific compositional paths (vertical sections). The software also supports liquidus surface projections, providing a comprehensive view of phase equilibria in complex multi-component systems. These features make it possible to analyze solidification paths and phase stability in greater detail.

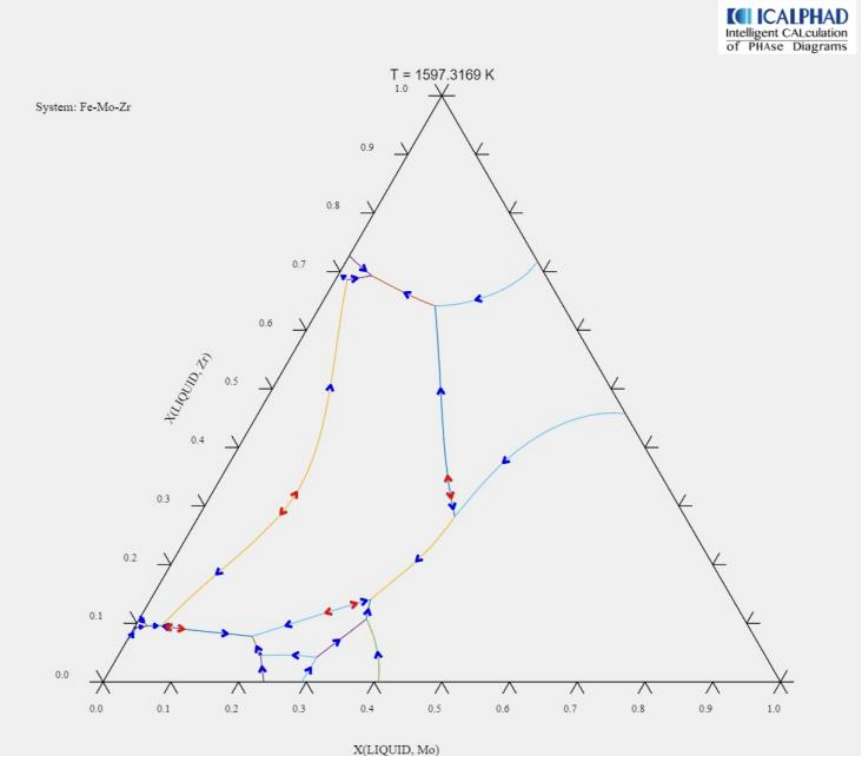

Figure 2. Fe–Mo–Zr liquidus projection calculated by using ICALPHAD software

2.3 Thermodynamic Property Calculations

Beyond phase diagram generation, ICALPHAD includes a thermodynamic property module. This allows calculation and plotting of fundamental properties such as Gibbs free energy, enthalpy, heat capacity, entropy, chemical potentials, and activities. The properties can be evaluated at both the system level and for individual phases, enabling detailed analysis of thermodynamic stability and reaction driving forces. High-resolution curves are automatically generated for visualization and export.

2.4 External Field Calculations

An advanced feature of ICALPHAD is its ability to model external field effects. For instance, modules have been implemented to calculate phase diagrams under applied magnetic fields, covering systems such as Fe-Co, Fe-Ni, and Co-Cr. These modules extend the software's applicability to emerging fields of functional materials design, where magnetic, electric, or stress fields strongly influence phase equilibria.

2.5 Optimization Framework

A distinguishing feature of ICALPHAD is its intelligent optimization framework. The framework employs a multi-objective approach, combining thermodynamic property data, two-phase equilibrium information, and invariant reaction data into a single optimization problem. A weighted sum method aggregates the different objectives, and the optimization is performed using the Barzilai–Borwein method, which provides rapid convergence while avoiding dependence on arbitrary initial parameter guesses[3]. This enables robust parameter optimization even when experimental datasets are incomplete, which is often the case in high-order systems.

2.6 User Interface and Workflow

The software is equipped with an intuitive graphical user interface (GUI) designed for usability in both research and engineering contexts. Users can:

Import database files (.TDB, .m, or other supported formats).
Select elements, phases, and parameter ranges via interactive panels.
Dynamically compute phase diagrams by adjusting temperature, composition, or pressure.
Visualize results in real time, including diagrams and thermodynamic property curves.
Export diagrams and datasets into multiple formats (e.g., PNG, PDF, CSV).

The GUI also integrates calculation logs and error reporting, which facilitate reproducibility and debugging. By automating routine steps such as parameter initialization and data parsing, ICALPHAD reduces the manual workload and minimizes user errors, ensuring a smooth workflow for both novice and expert users.

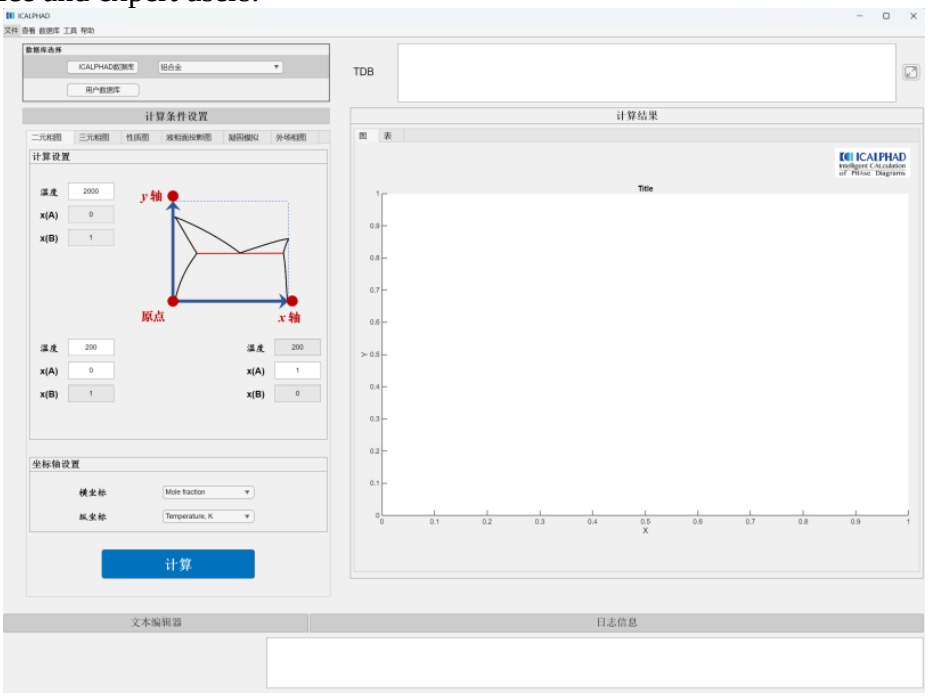

Figure 3. Graphical user interface of the ICALPHAD software

3. CONCLUSION

The ICALPHAD software provides an integrated platform for phase diagram calculation and thermodynamic property evaluation. By incorporating an intelligent multi-objective optimization framework, it achieves robust performance even with incomplete experimental data. With its modular design and user-friendly interface, ICALPHAD offers a reliable tool for computational thermodynamics, with potential for further extension to more complex systems.

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