CPDDB

Computational Phase Diagram Database

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計算状態図データベースでは、CALPHAD 法による熱力学解析により得られた各相のギブスエネルギー関数をまとめたデータベースファイル（TDB ファイル）を集録しています。この TDB ファイルと熱力学計算ソフトウェアを用いることで、各種熱力学量、相平衡、状態図を求めることができます。現在 500 種類以上の一元系、二元系、多元系合金状態図の TDB ファイルが集録されています。

CPDDB のご利用には MatNavi ユーザ登録が必要です。登録・ログインは https://cpddb.nims.go.jp/ から行ってください。

On Computational Phase Diagram Database, the Gibbs energy functions of the phases are accumulated in a form of TDB (Thermodynamic DataBase) files, which are obtained from the CALPHAD-type thermodynamic assessments. With the TDB files, various thermodynamic quantities, phase equilibria, and phase diagrams can be calculated on commercial thermodynamic software packages. The current database includes more than 500 unary, binary, and higher-order systems.

To use CPDDB, MatNavi user registration is required. For registration and log in, please go to https://cpddb.nims.go.jp/en/

About NIMS Thermodynamic Database

Introduction

The CALPHAD-type thermodynamic assessments of phase diagrams have been intensively performed in recent years. In the form of thermodynamic databases, the results of such assessments are, in general, made available to the scientific community [1,2]. However, there are still many of the assessments that have not been incorporated into these databases, nor have they been made available as database files suitable for use with Thermo-Calc [1] or PANDAT [2] calculations. Even if alloy systems are already included in existing databases, it does not mean that these data are exact and not subject to change. With new experimental data and using different thermodynamic models, the re-assessment of many alloy systems has been performed. Looking at the Cu-Zr system in the NIMS thermodynamic database, for example, five different thermodynamic assessments have been performed in the past, and two of these are available in commercial databases, while the recent assessments are not. Thus, one has to wait for the databases to be updated and the latest assessment becomes available. Another option is for the user to create a database file. However, this can be a difficult task since the user must check the thermodynamic models employed, sublattice configurations, parameters for pure elements, etc. Clearly, even though this depends on the alloy system, it is not a simple process and requires knowledge of commands in the thermodynamic software, thermodynamic models, and the CALPHAD-type assessments. Moreover, in some cases, since some papers have misprints of parameters and free energy expressions, an incorrect phase diagram may be obtained even if the correct commands were used to obtain the user database file. Thus, because of these difficulties some users do not attempt, or become frustrated with, such thermodynamic calculations. More importantly, these difficulties may discourage users from using the results of these assessments. In order to improve on or remove these difficulties, the NIMS thermodynamic database provides user database files and macro files for use with Thermo-Calc, where these files are ready-made for ease of use with thermodynamic calculation software. We believe that the NIMS thermodynamic database will encourage first-time users of thermodynamic assessments and provide accurate and reliable data to existing users.

Thermodynamic data in the NIMS thermodynamic database

The NIMS thermodynamic database consists of the TDB (Thermodynamic Database) file. One can use the TDB file on Thermo-Calc [1], PANDAT [2], CaTCalc [3], and open-source software such as OpenCALPHAD [4] and PyCALPHAD [5]. The TDB files have been tested mainly on PANDAT. Users should note that for different versions when the TDB files produce may error; please check the commands used in the files and change the syntax to match your version. If you have any questions, or there are misprints/errors found in these files, please contact the webmaster. Thermodynamic

calculation software [1-6] is necessary for calculations using the TDB files. For Fact-Sage [6] users, database conversion is necessary to use the TDB files. Please ask a distributor in your area.

References

[1] Thermo-Calc Software, http://www.thermocalc.se/
[2] PANDAT, http://www.materials-design.co.jp/
[3] CaTCalc, https://en.rictsystems.com/
[4] OpenCALPHAD, http://www.opencalphad.com/
[5] PyCALPHAD, https://pycalphad.org/docs/latest/
[6] FactSage, http://gtt-technologies.de/