19th INTERNATIONAL CONFERENCE ON DIFFUSION IN SOLIDS AND LIQUIDS
DSL2023
HERAKLION, CRETE | GREECE
26-30 JUNE 2023

ABSTRACT:

CALTPP: An Intelligent Program to Calculate Atomic Mobility and Diffusivity in Multicomponent Alloys

Yong Du, Shiyi Wen and Yuling Liu

State Key Laboratory of Powder Metallurgy, Central South University, Changsha, Hunan 410083, China

A program CALTPP (CALculation of ThermoPhysical Properties) is developed to provide temperature and composition-dependent thermophysical properties (diffusion coefficient, interfacial energy, thermal conductivity, viscosity, and molar volume) [1,2]. In the diffusion module, the measured composition profiles are directly used during the calculation of diffusivity by the novel numerical inverse approach and the corresponding atomic mobility parameters are extracted simultaneously. A robust computational framework to obtain accurate diffusion coefficients with the fewest mobility parameters for single-phase alloys is proposed. A general criterion for selecting mobility parameters of both binary and ternary interactions to be stored in kinetic databases were proposed for the first time. The thermal conductivity module includes a microstructure-based thermal conductivity model with key inputs from CALPHAD-type approach to obtain thermal conductivity for single-phase alloy [3] and two-phase composites [4], which enables the inverse design of material composition and structure from a given thermal conductivity. In addition, the models to describe interfacial energy, viscosity, and volume are also developed and implemented in CALTPP. It is expected that CALTPP will be an effective contribution in both scientific research and industrial application.

Keywords : CALTPP; Thermophysical properties; Diffusion; Thermal conductivity; Numerical inverse approach

References

[1] Y. Liu, Y. Du, S. Wen et al., J Mater Sci Technol, 42 (2020) 229-240.
[2] S. Wen, C. Du, H. Liu et al., J. Alloys Compd., 933, 167805-13 (2023).
[3] S. Wen, Y. Liu, Y. Du et al., J Mater Sci Technol, 59 (2020) 72-82.
[4] S. Wen, Y. Du, J. Tan et al., J Mater Sci Technol, 97, (2022) 123-33.