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

ABSTRACT:

Accurate Prediction of Diffusivities in Multicomponent Alloys from *ab initio*

X. Zhang1, S. V. Divinski2, B. Grabowski1

1Institute for Materials Science, University of Stuttgart, D-70569 Stuttgart, Germany
2Institute of Materials Physics, University of Münster, 48149 Münster, Germany

An indispensable complementary tool in understanding the observed diffusion phenomena is ab initio density-functional-theory (DFT) simulations. However, DFT simulations of diffusivities face significant challenges in multicomponent alloys. The well-established ab initio framework for pure metals and dilute alloys breaks down due to the significant chemical complexity that cannot be analytically simplified. To achieve accurate predictions that enable a quantitative comparison with experiment, among the key properties of vacancy-mediated diffusion, vacancy energetics depending on both configurational and vibrational degrees of freedom should be properly addressed. In this talk, we show that the configuration-dependent vacancy energetics in multicomponent alloys can be extracted from a special-quasirandom-structure-based statistical analysis via the configurational excitation mechanism. Vibrational contributions, particularly explicit anharmonic vibrations in both vacancy formation and migration, can be efficiently resolved with the aid of machine learning interatomic potentials.

[1] X. Zhang, S. V. Divinski, and B. Grabowski, Acta Materialia 227 (2022) 117677.
[2] A. Dash, A. Paul, S. Sen, S. V. Divinski, J. Kundin, I. Steinbach, B. Grabowski, and X. Zhang, Annual Review of Materials Research 52 (2022) 383–409.