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Prediction and Modeling of Atomic Mobility in Alloys ZI-KUI LIU, Department of Materials Science and Engineering, The Pennsylvania State University — Atomic diffusion is a common and important non-equilibrium process in solids that takes place at finite temperatures. To computationally simulate atomic diffusion processes, the thermodynamic and atomic mobility databases of the materials of interest are needed. The modeling technique of atomic mobility databases and related software has been becoming more and more matured in the last decades. However, the input data for the modeling is exclusively taken from experimentally measured tracer and chemical diffusion coefficients. In this presentation, our recent progress in predicting self and dilute diffusion coefficients by quantum mechanics calculations will be discussed [1]. Our approach to the unstable vibrational mode of transition states during diffusion will be presented. The contribution to phenomenological modeling of atomic mobility will be briefed.

[1] M. Mantina, Y. Wang, R. Arroyave, L. Q. Chen, Z. K. Liu and C. Wolverton, "First-principles calculation of self-diffusion coefficients," Phys. Rev. Lett., Vol.100, 2008, 215901.

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