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Ab Initio Calculations of Transport in Titanium and Aluminum Mixtures[1] NICHOLAS WALKER, BRIAN NOVAK, KA MING TAM, DOREL MOLDOVAN, MARK JARRELL, Louisiana State Univ - Baton Rouge — In classical molecular dynamics simulations, the self-diffusion and shear viscosity of titanium about the melting point have fallen within the ranges provided by experimental data. However, the experimental data is difficult to collect and has been rather scattered, making it of limited value for the validation of these calculations. By using ab initio molecular dynamics simulations within the density functional theory framework, the classical molecular dynamics data can be validated. The dynamical data from the ab initio molecular dynamics can also be used to calculate new potentials for use in classical molecular dynamics, allowing for more accurate classical dynamics simulations for the liquid phase. For metallic materials such as titanium and aluminum alloys, these calculations are very valuable due to an increasing demand for the knowledge of their thermophysical properties that drive the development of new materials. For example, alongside knowledge of the surface tension, viscosity is an important input for modeling the additive manufacturing process at the continuum level. We are developing calculations of the viscosity along with the self-diffusion for aluminum, titanium, and titanium-aluminum alloys with ab initio molecular dynamics.

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