Diffusion Properties of metallic liquids and their binary alloys

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Liquid diffusion coefficients are key input parameters for modelling of solidification as well as important parameters for testing potentials used in molecular dynamics simulations. It has been shown that the simulated microstructure of a material sensitively depends on the diffusion coefficient [1]. Further it has been shown for a pure metal, Ti, that diffusion coefficients can be used to improve molecular dynamics simulations [2]. However, diffusion data for liquids are scarce compared with data available for solids and show typically a large error when obtained with conventional capillary experiments [3]. Consequently, the relation between self-, impurity and chemical diffusion in liquids, their temperature dependence, and their relation to thermophysical properties such as viscosity are still debated.

A comprehensive data set on self-, impurity, and chemical diffusion coefficients for pure metals, liquid Ge, and Al-based alloys is presented. Neutron time-of-flight spectroscopy was used to determine self diffusion coefficients with high accuracy whereas x-ray radiography in combination with capillary experiments was used to determine accurate impurity and interdiffusion coefficients in binary alloys. For liquid-Ge and liquid-Al it is shown that impurity diffusion coefficients do not depend on mass. For liquid-Ge a dependence of impurity diffusion on the covalent radius of the impurity atom is observed and impurity diffusion and solvent self-diffusion agree within error bars. At and around the melting point diffusivities are typically well described by an Arrhenius law. It is shown that the Stokes-Einstein relation predicts diffusivities based on viscosity data only within a factor two for pure liquid metals. Finally, measured interdiffusion coefficients for Al-Cu alloys are compared with calculated values using the empirical Darken relation and measured Cu self diffusion coefficients. These data are discussed in the context of recent findings by molecular dynamics simulations.

References

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