The Role of the Interface in Thermomigration in Alloys

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Thermomigration in alloys is important in numerous processes in which thermal gradients are present, such as in nuclear reactors, gas turbines, or electronic interconnects. Recently, the migration of liquid enclosures of germanium rich phase in a solid matrix of a silicon rich phase has been observed [1], opening new avenues for material design. In order to obtain a description of thermomigration, factors such as atom diffusivity and heat of transfer have to be known, which are generally scarce [2]. Even more elusive are such parameters for interfaces between two phases. Recently, it has been shown for Si and Ge that the interface can be treated as an autonomous thermodynamic system [3], leading to well defined interface properties. In the present contribution, we report conditions during melting of Si, in a first attempt to determine the interface transport coefficients. We follow the procedure established for liquid-vapor transition of Lennard-Jones particles [4]. A Kapitza resistance is expected from the literature (Healey), the mass transfer coefficient and coupling coefficient are unknown. The coefficients for the pure component are functions of the interface temperature only, when the interface is flat. The aim is to eventually determine the diffusivity and heat of transfer for Si/Ge in bulk and at the solid-liquid interface using non-equilibrium molecular dynamics (NEMD). Subsequently, these parameters can be employed in mesoscale numerical models of thermomigration in Si [Ge alloys, comparing models that treat the surface explicitly with those that don't.

References:

[1] U. Gibson, private communication.

[2] R. R. Mohanty, J. E. Guyer, Y. H. Sohn, J. Appl. Phys. 106, 034912 (2009).

[3] R. Rurali et. al., Phys.Chem.Chem.Phys., 18, 13741, (2016)

[4] S. Kjelstrup, D. Bedeaux, *Non-equilibrium thermodynamics of Heterogenous Systems*, Singapure: World Scientific, (2008)