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Atomistic Structure and Energy of Solid-Liquid Interfaces

WAYNE KAPLAN, Technion - Israel Institute of Technology

As microstructural length-scales are reduced, the role of interfaces in determining the properties of materials becomes more dominant. The importance of the correlation between interface structure and chemistry with interface (and bulk) properties is evident in a range of material systems, and is a topic of intense experimental and theoretical work for solid-solid interfaces. While detailed thermodynamic analysis of solid-liquid interfaces is routinely conducted, knowledge of the local structure at solid-liquid interfaces is still incomplete. To be more specific, the correlation between the structure of the solid, and the structure in the liquid near the interface, has not been fully addressed. In this presentation, in-situ ($\sim$750 $^\circ$C) high resolution transmission electron microscopy (HRTEM) of liquid Al in contact with sapphire (α-Al_2O_3) will be presented. Contrast perturbations in the liquid Al adjacent to the crystalline substrate were determined to be due to ordering of the liquid, via detailed multi-slice dynamic electron scattering simulations. Details on the type of ordering were interpreted by molecular dynamics simulations of liquid Al in contact with crystalline substrates, and compared to sessile drop studies of liquid Al on sapphire. These results are compared with recent HRTEM investigations of equilibrium amorphous films at metal-Al_2O_3 interfaces, where partial ordering of the film plays an important entropic role in reaching stable nanometer-thick films. This will then be extended to equilibrium segregation, and the concept of extremely small volumes of liquids confined by crystals.