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Effect of Mg doping on the Structure and Reflectivity of Alumina surfaces TIMOTHY PENNYCOOK, Vanderbilt University, JUAN C. IDROBO, Vanderbilt University and Oak Ridge National Laboratory, KALMAN VARGA, Vanderbilt University, SOKRATES T. PANTELIDES, Vanderbilt University and Oak Ridge National Laboratory — Mg is used in the fabrication of Al alloys to increase the strength of the material. In typical applications, a layer of alumina is present on the surface. The high diffusivity and chemical reactivity of Mg means that Mg can migrate from the bulk alloy to the alumina film and the surface, where it can affect the structural and optical properties of the material. The doping of Al alloys with Mg is known to cause "darkening" and affect the coloration of the material. We will report results of first principles density functional theory calculations that explore the segregation modes of Mg in the near-surface region of alumina and the corresponding effect on optical properties, *i.e.*, reflectivity. This work is supported in part by NSF grant DMR-0513048 and ALCOA Inc.

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