Incoherent Imaging of Atoms at Interfaces

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Z-contrast scanning transmission electron microscopy combined with electron energy loss spectroscopy provides an essentially complete atomic-scale characterization of interfaces, including atomic structure and impurity segregation sites, concentration and valence. Such data is a perfect starting point for first-principles theoretical calculations, which provide total energies, diffusion pathways, activation barriers, and the link to properties. For As in Si, images show segregation in particular atomic columns in a grain boundary, and calculations show the As to be in the form of dimers. In MgO, an impurity-induced structural transformation has been revealed. At the Si/SiO_2 interface, the structure of the last crystalline plane is seen directly in the image, and composition profiles show substantial sub-stoichiometric oxide. Theory shows that abrupt interfaces are energetically preferred, and suggests the origin of dangling bonds. In catalysis, *Z*-contrast images show preferred configurations of atomically-dispersed Pt and Rh. Theory reveals a remarkably complex situation, that γ-alumina is a sequence of hydrogen containing compounds with H exchanged with surface Al in a dynamic fashion, and explains the atomic sites and configurations observed experimentally.

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