Si/Cu Interface Structure and Adhesion

XIAO-GANG WANG, JOHN SMITH, Delphi Research Labs — An *ab initio* investigation of the Si(111)/Cu(111) interfacial atomic structure and adhesion is reported [1]. Misfit dislocations appear naturally, as do hcp interfacial silicide phases that vary with temperature. The silicides form in the interface even at relatively low temperatures. These results are consistent with available experimental data.