Delamination Nanomechanics at Organosilane-tailored Copper-Silica Interfaces

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ABSTRACT

Quantifying the contribution of energy dissipating mechanisms to the interface fracture toughness is crucial to develop a fundamental atomistic understanding of interface fracture. Isolating the contribution of plastic deformation γ_p from interfacial toughness Γ_{FT} is limited by uncertainties in crack path, fracture surface area, type and number of bonds broken, and plastic deformation occurring in either layers. Current descriptions of interfacial toughness neglect either plasticity (brittle fracture) or adhesion (ductile fracture) towards interfacial toughness. However, these models fail to provide atomistic descriptions of fracture at interfaces comprised of both brittle and ductile materials, i.e., where γ_a *and* γ_p are comparable and neither term can be neglected.

This study investigates experimental quantification of the contributions of the work of adhesion γ_a and plastic dissipation energy γ_p to the fracture toughness Γ_{FT} of a model copper-silica interface with an organosilane monolayer. This model system overcomes prior experimental uncertainties by constraining fracture to occur in a nanoscopically confined plane via exclusive siloxane bond fissure at the interface. Siloxane bridges are susceptible to hydrolysis; hence varying the water activity a_{H_2O} provides a facile means to tune the interfacial strength – validated by density functional theory calculations. This approach also allowed us capture the onset of copper film plasticity providing a direct method to quantify flow stress σ_y for confined thin copper film. A 7-fold increase in the Γ_{FT} was observed by increasing the thickness of the copper layer from 25 to 165 nm, and γ_p was measured as a function of γ_a which had only been done by modeling earlier. The study also determines the effect of temperature on the distribution of fracture energy into plasticity and adhesion.

Our methodology of altering γ_a by manipulating a single type of bond in an interfacial molecular nanolayer through environmental control can help obviate errors in estimating fracture toughness arising from neglecting plasticity or adhesion. This framework may be adapted for studying other bimaterial systems through the use of molecular layers with appropriate termini and thus paves the way for rational design and accurate reliability modeling of materials and structures comprised of heterointerfaces, e.g., composites, coatings, material joints, nanoelectronics devices and packaging.