An Atomistic Level Investigation into the Strength of Polymer/Metal Interfaces

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Abstract

Polymer/metal interfaces are ubiquitous. They can be found in numerous engineering applications. For example, polymers are used as adhesives and coatings for metals in aircrafts, automobiles, microelectronics, MEMS, and polymer composites are routinely used for retrofitting damaged structures. Of particular interest to this project is the need for the miniaturization of microelectronic devices, which has led to the emerging technology of 3D packaging, in which numerous metal layers are bonded together by polymer dielectric adhesives. The reliability of microelectronics devices (cell phone, computers, *etc.*), to a large extent, depends on the integrity of these material interfaces, because they are often the "weakest links", and their failure often leads to the malfunction of the entire electronics device. Therefore, understanding the structure-performance relationship of polymer/metal interfaces is critical in designing, building and operating the next generation structures, components, devices.

In this paper, we present some recent results on the structure-performance relationship in polymer/metal interfaces. In particular, cross-linked epoxy/Cu interfaces were investigated using both full-atomistic and coarse grained molecular dynamic simulations. A significant advantage of the coarse-grained model is its ability to simulate bond breakage, which enables the simulation of polymer failure. Taking advantage of this new capability, we simulated the deformation and failure of epoxy/Cu interfaces. Our results show that, upon loading, deformation in the epoxy is highly localized to a thin layer near the Cu substrate. Such localized deformation facilitates the definition of an interfacial zone based on the deformation inhomogeneity, from which a cohesive zone law can be extracted. Also investigated were details of microstructure evolution including cavitation and polymer chain stretching/scission within the interfacial zone. In addition, effects of strain rate, temperature and epoxy molding compound's cross-link density were studied.

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Jianmin Qu, Walter P. Murphy Professor in the McCormick School of Engineering and Applied Science at Northwestern University, received his Ph.D. in Theoretical and Applied Mechanics from Northwestern University. Before joining the faculty at his alma mater in 2009, Professor Qu was on the faculty of the School of Mechanical Engineering at the Georgia Institute of Technology from 1989 to 2009.

Professor Qu's research focuses on several areas of theoretical and applied mechanics including micromechanics of composites, interfacial fracture and adhesion, fatigue and creep damage in solder alloys, thermomechanical reliability of microelectronic packaging, defects and transport in ionic solids with applications to solid oxide fuel cells and batteries, and ultrasonic nondestructive evaluation of advanced engineering materials. He has authored/co-authored two books, 10 book chapters and over 160 referred journal papers in these areas.