Multi-scale simulation of degradation in electric contact materials

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Interfacial degradation of metal/metal electrical contacts limits the performance of many modern devices. Often this degradation process occurs through mechanical wear due to sliding or through repetitive open and close cycles. The nature of mechanical wear due to cold welding followed by de-adhesion is a complicated process under ambient conditions. Obtaining an understanding of the degradation process is more challenging when voltage is applied due to enhanced heating and the local thermal profile. In an effort to understand this process with atomic resolution, we have developed a multi-scale method that simultaneously solves electric and thermal transport equations and couples this information to an underlying molecular dynamics simulation. This method allows for the application of appropriate thermal conditions in the vicinity of the contact as well as the extension of the length scale of the simulation. This talk will present details of the method as well as its application to two systems of interest. The first system is a normally loaded and/or sliding Al/Cu single asperity contact with no voltage, constant voltage, or constant current. The second system is an Au/Au single asperity contact with and without an applied voltage. The understanding obtained from these simulations can be applied to predict degradation behavior in hot and cold switching radio frequency micro-electrical mechanical systems.