Modeling and Characterization of Aging and Reliability of Si NWs

Silicon (Si) nanowires (NWs) have drawn the interest of many researchers since the first research was carried out fifty years ago. They are of interest for use as building blocks in the bottom-up assembly of nanoscale devices and circuits due to their exceptional electrical and mechanical properties. Devices and circuits using Si NWs that have been demonstrated include field-effect transistors, biological and chemical sensors, logic circuits, thin film transistors and address decoders. Our research goal is to predict the lifetime and reliability of nanoscale materials, and is motivated by the fact that, to-date, there is very limited research on material aging at the nanoscale. However, preliminary research by the PIs indicates that even with as little as 30 min of aging in an extreme environment, a Si NW will undergo significant changes in diameter and oxide layer thickness. To achieve this goal, we are focusing our efforts on developing and validating an aging protocol for Si NWs and studying the resulting changes in material properties. Our specific research objectives are: (1) Test the hypothesis that extreme environments can be used to age NWs with experimental testing and validate of an aging protocol on Si NWs that is flexible for NWs in general; (2) Study compositional changes of the surface and bulk portions of the Si NWs with high resolution transmission electron microscopy (TEM) and scanning tunneling electron microscopy (SEM) and correlate this to atomistic modeling of the compositional changes and predictions of the elastic behavior and properties; (3) Accurately measure (within 5% uncertainty) the elastic modulus and fracture strength of Si NWs aged in an extreme environment; (4) Accurately predict the conditions under which a Si NW's elastic properties exhibit mechanical changes above 20% (the applied definition of failure) due to aging; (5) Establish, using atomistic simulations, the temperature-dependent structure-property relationships governing the elastic and inelastic mechanical behavior, properties and eventually performance degradation of oxide covered Si NWs.