ABSTRACT

Surface dominated nanostructures such as nanowires have recently garnered significant attention due to their unique physical properties. In this presentation, I will discuss both atomistic and multiscale modeling effects, in conjunction with targeted experimental studies, that elucidate surface effects on the mechanics of crystalline nanowires.

Using atomistic modeling, I will discuss recent predictions of novel shape memory and pseudoelastic behavior observed in FCC metal nanowires that are not observed in the corresponding bulk materials. I will discuss the important role of nanoscale surface stress effects in enabling the shape memory response, and I will discuss the novel atomistic deformation mechanisms that are observed during the mechanical deformation of shape memory nanowires. I will also present recent experimental results that confirm part of the shape memory response via twin-mediated superplasticity of gold nanowires.

The second part of the talk will discuss recent developments in multiscale, finite element method-based modeling to capture surface effects on the mechanical behavior and properties of both FCC metal and semiconducting nanowires. I will discuss this approach, the surface Cauchy-Born model, then demonstrate its ability to capture size, surface and boundary condition effects on the elastic properties of the nanowires. Specific attention will be made to compare the obtained results to those where surface effects are neglected such that an understanding of how surface effects impact the elastic properties of nanowires across various length scales can be obtained.