Current research in Prof Gao’s research group is focused on nanomechanics of engineering and biological systems. For engineering systems, they use molecular dynamics simulations and continuum modeling tools to study deformation, diffusion, growth, grain boundaries, stress evolution and failure in thin films and nanocrystalline materials. For biological systems, they use continuum mechanics, statistical mechanics and atomistic simulations to study how biological materials such as bone, gecko and cell achieve their mechanical robustness through structural hierarchy. The critical issues under investigation include stiffness, toughness, contact, adhesion, viscoelasticity, diffusion, size effects, convergent evolution, flaw tolerance, optimal shape, aspect ratios, self-assembly, endocytosis, etc.

In this talk, Prof Gao will discuss some recent studies on the mechanics of plastic deformation in nanocrystalline materials as well as mechanics of focal adhesions in cell-substrate interactions. One study attempts to explain recent experiments that plastic strains in nanocrystalline aluminum and gold films with grain sizes on the order of 50 nm are partially recoverable. To reveal the mechanisms behind such strain recovery, we perform large scale molecular dynamics simulations of plastic deformation in nanocrystalline aluminum with mean grain sizes of 10, 20, and 30 nm. Our results indicate that the inhomogeneous deformation in a polycrystalline environment results in significant residual stresses in the nanocrystals. Upon unloading, these internal residual stresses cause strain recovery via competitive deformation mechanisms including dislocation reverse motion/annihilation and grain-boundary sliding/diffusion. Our analysis shows that, even under strain rates as high as those in molecular dynamics simulations, grain boundary-mediated processes play important roles in the deformation of nanocrystalline aluminum. The second topic attempts to explain recent experiments that cells can strongly sense mechanical properties of their surroundings. We consider clusters of specific receptor-ligand bonds that link an animal cell to an extracellular matrix. To understand the mechanical responses of cell adhesions, we develop a stochastic-elasticity model of a periodic array of adhesion clusters between two elastic media subjected to inclined loads, in which stochastic descriptions of molecular bonds and elastic descriptions of interfacial traction are unified in a single modeling framework. The results show that elasticity can play a key role in cell-substrate adhesion by modulating the lifetime of focal adhesions across many orders of magnitude. The predictions of our model provide feasible explanations for a wide range of experimental observations.