Mechanical Bending of Nanoscale Thin Films:
Dominating Role of Atomic Surface Reconstruction and Intrinsic Surface Stress

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Fundamental understanding of mechanical bending of nanoscale thin films have important implications in many areas of nanotechnolgy, such as nanoelectromechanical systems, nanomechanochemical sensors, strain induced self-assembly of nanostructures, and flexible electronics. I this talk, I report our recent work on atomistic simulations and theoretical analyses of bending of nanometer-thick silicon (Si) and silicon/germanium (Si/Ge) films, revealing the dominant role of atomic surface reconstruction and intrinsic surface stress in governing the bending behavior of nanoscale thin films. We show that a Si nanofilm may bend itself under its own intrinsic surface stress due to surface reconstruction without applying external stress, and a bilayer Si/Ge nanofilm may even bend toward the Ge side, opposite of the bending direction defined by misfit strain. We further show that the bending curvature of nanofilms does not simply follow the classical Stoney and Timoshenko formula. These findings demonstrate that the mechanical bending of nanoscale thin films can be *qualitatively* different from that of micro and macroscopic thick films.