Atomistic Investigation of Size and Temperature Effects on the Compressive Behavior of Cracked Silicon Nanopillars

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The performance, sensitivity, and reliability of many MEMS and NEMS devices are directly governed by the mechanical behavior of their structural components. Silicon nanobeams and nanopillars are widely used in MEMS and NEMS devices as sensors and actuators. These structures must function reliably under varying thermal conditions, from low to elevated temperatures [1]. Experimental and atomistic simulations have shown that the mechanical response of silicon nanostructures is size-dependent [2]. This size-dependent behavior is further influenced by temperature and structural defects such as cracks [3]. Therefore, it is essential to investigate the size-dependent mechanical response of silicon nanostructures under the combined effects of crack defects and temperature variations.

In this study, molecular dynamics (MD) simulations are used to investigate the compressive behavior of cracked silicon nanopillars across a range of sizes and temperatures. Particular attention is given to how crack defects influence buckling loads. The atomistic results are compared with continuum-based models reported in the literature. The findings show that current continuum models fail to accurately capture the size-dependent compressive response of cracked silicon nanopillars. The underlying physical mechanisms responsible for these discrepancies are analyzed. In particular, the analysis reveals that conventional kinematic continuity conditions used to model cracked cross-sections may not be valid at the nanoscale and require further refinement.

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