

# Ductile-to-fragile transition in compressed amorphous silicon nanopillars by numerical simulations

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Nanopillars are emerging nanostructures that have attracted much attention in the last years for their applications in different fields, such as nanoelectronics and nanobiotechnology. Therefore their mechanical properties are very important and need to be understood. Previous studies have already reported a brittle to ductile transition as a function of the nanopillar's diameter, but contradictory results have been found for different systems: a ductile behavior has been observed when decreasing the size of crystalline silicon nanopillars [1] and metallic glass nanowires [2] while an opposite trend has been reported for crystalline silicon nanowires with an amorphous shell [3]. Here we address the mechanical behavior of amorphous silicon nanopillars by Molecular Dynamics simulations in the quasi-static limit. We show that the mechanical properties of the a-Si nanopillars strongly increase by increasing the nanopillar's diameter. We also observe that the internal pressure of the sample decreases with the nanopillar's diameter following a power law with an exponent depending on the aspect ratio of the nanopillar. In order to get a deeper understanding of the mechanical behavior we perform a microscopic analysis of the plastic rearrangements occurring in the nanopillar. This analysis suggests that the plastic rearrangements are initiated near the surface of the nanopillar in the elastic regime, and then propagate in the bulk at larger strains. Furthermore this behavior can be ascribed to the propensity of plastic rearrangements to localize near structural defects at the surface for small strains, and then to move closer to defects in the bulk at large strains. This work opens the door to the possibility of playing in a controlled manner with the microstructure to control the initiation and propagation of plasticity.

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