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SURFACE EFFECTS ON MECHANICAL PROPERTIES AND INSTABILITY OF FCC NANOWIRES AND NANOFILMS

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We employed molecular statics and density functional theory simulations to study effects of surface on mechanical properties and instability behaviours of FCC nanowires and nanofilms under uniaxial loading. For FCC [100]/(001) nanowires under tension, it is found that the existence of surfaces delays the critical strain of instability. As the nanowire thicker, the critical strain decreases and approaches that of the bulk counterpart. Bifurcation, which is the deformation mode of the bulk material at the onset of instability, is still observed in nanowires, but the amount of contraction and expansion are reduced with decrease of the nanowire thickness. For metal nanofilms, compressive forces induced by (001) free surface, together with phase transformation induced by the instability of cubic materials are the factors leading to negative Poisson's ratio behaviour in the (001) nanofilms.