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Hypothetical Silicon Nanotubes under Axial Compression

강정원, 황호정
중앙대학교 기술과학연구소 및 전자전기공학부

This study showed the response of silicon nanotubes (SiNTs) under axial compression using an atomistic simulation based on the Tersoff potential. A pressure, proportional to the deformation within Hooks law, eventually led to a collapse of the SiNT and an abrupt change in structure. Using the sum of the cross sections of atoms on the cross section of SiNT and pressure on SiNT, we determined Youngs modulus of SiNTs that was constant irrespective of the diameter of SiNTs. As the diameter of SiNTs increased, the collapse pressure, that is to say the critical stress linearly decreased. However, net forces on SiNTs occurring their collapse were almost constant irrespective of the diameter of SiNTs. We also calculated the variations of the volume of unit cell as a function of pressure that were not dealt with in previous works that considered carbon nanotubes under compression. With properly chosen parameters of SiNTs (Youngs modulus, effective spring constant, diameter, lattice constant, and cylindrical volume modulus), the critical strain, the collapse pressure, the elastic energy, and the critical volume at which the buckling events of SiNTs occur can be estimated by equations induced by this work.