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A Study on III-Nitride Nanotubes based on the Tersoff Potential

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We have investigated the structural and the mechanical properties of single-wall III-N nanotubes using atomistic simulations and the Tersoff-type potential. The Tersoff-type potential for III-N has been effectively described the properties of III-N nanotubes, such as the bond length, the diameter, and the curving strain energy of sheet-to-tube. Nanomechanics of III-N nanotubes under the compression loading were investigated and the calculated Youngs moduli of III-N nanotubes were lower than that of CNT. The cohesive energies per atom for AlN nanotubes were higher than that for the cubic AlN bulk, and this implies the difficulty in producing AlN nanotubes or graphite-like sheets. However, since the elastic energy per atom to curve the sheet into cylinder for AlN is very low, if graphite-like sheets of AlN are formed, the extra cost to produce the tubes is very low.

Since we have investigated the nanomechanice of only (5, 5) III-N nanotube, systematic analysis for III-N nanotubes could not be achieved. Therefore, further investigations on III-N nanotubes will include studies on the systematic analysis for thermal and mechanical properties using a molecular dynamics simulation.