산화아연 나노선과 나노튜브의 구조 및 탄성계수에 관한 원자단위 연구

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Atomistic simulation of structural and elastic modulus of ZnO nanowires and nanotubes

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Abstract : The structural stability and the elastic modulus of hexagonal ZnO nanowires and nanotubes are investigated using atomistic simulations based on the shell model. The ZnO nanowire with (10-10) facets is energetically more stable than that with (11-20). Our calculations indicate that the structural change of ZnO nanowires with (10-10) facets is sensitive to the diameter. With decreasing the diameter of ZnO nanowires, the unit-cell length is increased while the bond-length is reduced due to the change of surface atoms. . Unlike the conventional layered nanotubes, the energetic stability of single crystalline ZnO nanotubes is related to the wall thickness. The potential energy of ZnO nanotubes with fixed outer and inner diameters decreases with increasing wall thickness while the nanotubes with same wall thickness are independent of the outer and inner diameters. The transformation of single crystalline ZnO nanotubes with double layer from wurtzite phase to graphitic suggests the possibility of wall-typed ZnO nanotubes. The size-dependent Young's modulus for ZnO nanowires and nanotubes is also calculated. The diameter and the wall thickness play a significant role in the Young's modulus of single crystalline ZnO nanowires and nanotubes, respectively.

Key Words : Atiomistic simulation, ZnO nanowires and nanotubes, elastic modulus