Lattice Vibrational Modes in Si/Ge Core-shell Nanowires

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We present a first-principles study on lattice vibrational modes of Si/Ge core-shell nanowires (NWs). We particularly focus on two types of modes of broad interest, the high-frequency optical modes and the radial breathing mode (RBM). Those optical modes exhibit substantial energy shifts as the structure of core-shell NWs varies, which can be attributed to the change of the strain condition. Moreover, those studied optical modes and their energy shifts are significant in the calculated Raman scattering spectrum, providing a convenient way to detect the structural information of core-shell nanomaterials. Meanwhile, the frequency of the RBM also strongly depends on the structure of core-shell NWs, which can be explained by an elastic media model. In particular, we find that the difference between sound velocities of core and shell are enhanced by the internal strain, which could be useful for thermoelectric applications based on core-shell nanostructures.

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