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Lattice Vibration in Silicon Nanowires LI YANG, XINYUAN ZHAO, M.Y. CHOU, School of Physics, Georgia Institute of Technology — The lattice vibrations for silicon nanowires along the [110] direction are investigated by first-principles calculations. The distribution of phonon modes at the Γ point is obtained for nanowires of various diameters. Two different frequency shifts are found for the optical modes and the collective modes, respectively. When the size of nanowires decreases, the frequencies of optical modes are red-shifted, while the frequencies of collective modes are blue-shifted. We provide an explanation for these trends based on a different quantum confinement effect. In addition, the controversy over clamped and free boundary conditions is resolved in light of our first-principles calculations. Finally, the relative Raman scattering activity in a small nanowire is evaluated. Based on these Raman modes, a practical method to estimate the size of nanowires is presented. We also find that quantum confinement considerably changes the sound velocity, which has a significant effect in the studies of transport properties in nanostructures.

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