Atomistic Studies of the Vibrational Properties of Fivefold Twinned Nanowires

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Fivefold twinned nanowires have attracted much attention in recent years due to their peculiar twinned microstructures and unique mechanical properties. These structures have great potential applications as active components in nano devices. In this work, the vibrational properties of fivefold twinned nanowires have been investigated by using molecular mechanics and molecular dynamics methods, including the transverse, longitudinal and torsional vibration. The frequency response and the fundamental vibration frequency of fivefold twinned nanowires under different vibrational directions have been obtained by performing fast Fourier transformation analysis of the potential energy *vs*. time. The length and radius dependencies of the fundamental vibration frequency have been studied and the applicability of the classic elastic vibration theory with effective material properties to nanoscale has been discussed. This work has been supported by the NSFC (11272003, 11232003), the 111 Project (B08014), the 973 Program (2010CB832704, 2011CB013401) and the Fundamental Research Funds for the Central Universities.

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