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Talk Invited Invited Talk

Vibrational Behavior of Metal Nanowires under Tensile Stress

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We have investigated the vibrational density of states (VDOS) of ultrathin Cu nanowires with $< 100 >$ and $< 111 >$ axial orientations and considered the effect of axial strain. The VDOS are calculated using a real space Green's function approach with the force constant matrices extracted from interaction potential based on the embedded atom method. Results for the vibrational density of states of a strain-free nanowire show quite distinctive characteristics compared to that of a bulk atom, the most striking feature of which is the existence of high frequency modes above the top of the bulk spectrum. Taking the specific example of the 5×5, H5 types and pure Cu nanowires at their 0K ground state configurations, we show that the existence of high frequency modes above the top of the bulk phonon spectrum is a reflection of the reduced dimensionality of the system rather than being an end effect of contamination or temperature. Through the projection of the total VDOS on local atoms of the wire, we identified the leading contributors to the enhancement of the modes at low and high frequencies: while the anomalous low frequency modes are primarily moderated by corner atoms, the aberrant high frequency modes are dominated largely by center atoms. In contrast to the case of helical nanowires, the existing aberrant high frequency modes shift to higher frequencies upon stretching the nanowire. However, the vibrational behavior at low frequencies remains almost the same with increasing axial strain. We, additionally, find that while the high frequency band above the top of the bulk phonon shifts to higher frequencies, the characteristics at low frequencies remains almost the same upon stretching the nanowire along the axial direction. More interestingly, these characteristics are found to be independent of the axial direction of the wire.

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