Surface phonon dispersion of Bi_2Se_3(111): evidence for a prominent surface acoustic wave

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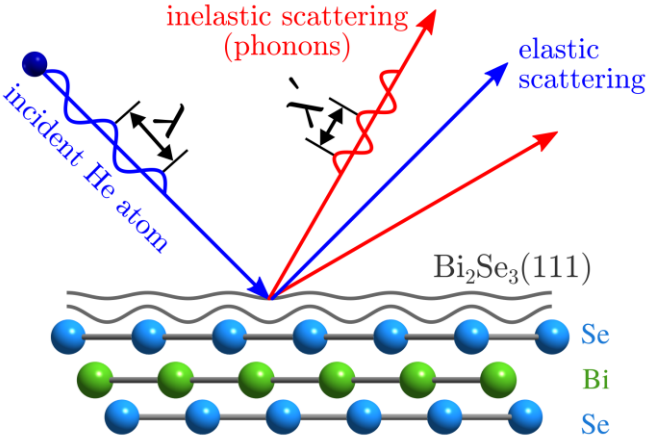
We present a combined experimental and theoretical study of the surface vibrational modes of the topological insulator Bi_2Se_3 [1]. Using inelastic helium atom scattering [2] we are able to resolve the acoustic and optical phonon modes of Bi_2Se_3(111) up to energies of 18 meV. The low energy region of the surface phonons is mainly dominated by the Rayleigh mode which has been claimed to be absent in previous experimental studies [3]. On the other hand, the appearance of the Rayleigh mode is consistent with previous bulk lattice dynamics studies as well as theoretical predictions of the surface phonon modes [4,5]. However, our results do not support the presence of a Kohn anomaly, connected with a surface phonon mode, as inferred from a previous experimental study [3].

The speed of sound of the Rayleigh mode is determined to be $v=(1561\pm44)\ \mathrm{ms}^{-1}$ from the experimental data. Comparison of the experimental data with the surface phonon dispersion as calculated by density functional perturbation theory shows excellent agreement. Moreover, there appear additional branches in the gap below the Rayleigh wave branch which cannot be attributed to any possible phonon branch of the ideal surface based on the calculations. The recent observation of dynamical charge density wave excitations on the semimetal Sb(111) [6] as well as in cuprate superconductors [7] suggests the assignment of these additional low-energy excitations to phason-amplitudon pairs.



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