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Structure and Phonon Dispersion of Bi(111) from He Atom Scattering

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As a material with significant differences in bulk and surface properties, bismuth (Bi) has attracted renewed interest among researchers. The presence of metallic surface states is unusual for a bulk semimetal and provides the playground for ideas related to the electronic response of the surface and even the possibility of two-dimensional superconductivity [1].
With regard to phonon states, calculations of the bulk phonon dispersion are consistent with experimental data only when spin-orbit interaction is taken into account [2]. Recently, squeezed bulk phonon states were measured with femtosecond x-ray diffraction [3].
In contrast to phonons in the bulk and the electronic surface structure nothing is known about the surface phonons of the Bi(111) surface. They are in a low energy region of meV and therefore not accessible with satisfying resolution for most scattering techniques, but with experiments using helium atom scattering (HAS) surface phonons can be investigated successfully.
We have used elastic and inelastic HAS to study the Bi(111) surface therefore we are able to present the first report on phonon creation and annihilation events on this surface. The surface phonon dispersion relation has been determined from measured time-of-flight spectra of inelastically scattered He atoms. The obtained group velocity lies somewhat above the bulk group velocity. Elastic HAS experiments reveal rather large diffraction peaks in comparison to other metals. A first comparison between theoretical (eikonal approximation, GR-method) and measured diffraction peak intensities yields a surface charge density corrugation of 16% of the surface unit cell. This value is surprisingly large since the reported metallic character of the Bi(111) surface would imply a nearly flat corrugation. The observed surface corrugation and the steep slope in the phonon dispersion may both point to the important role of the strong covalent bonds at the surface.

REFERENCES

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