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Investigation of surface phonons by inelastic helium atom scattering of the Bi(111) surface

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The remarkable differences between its bulk and surface properties make the semimetal Bismuth (Bi) an interesting candidate for the investigation of surface phonons, because in contrast to the bulk not much is known about their behaviour. [1] With the strictly surface sensitive technique of inelastic helium atom scattering (HAS) the observation of these quanta of lattice vibrations on the surface is possible.

Since first results of our measurements were published in [2], additional data was gained with enhanced data analysis and new measurements:

Time-of-flight (TOF) spectra using HAS from the (111) surface of a Bi single crystal at room temperature, which were used for determining the surface phonon dispersion curve, were reviewed with improved algorithms reducing the noise level on the phonon-creation side of the spectra. Additional peaks were revealed, which were analyzed for their possible origin in excited surface phonons in acoustical or optical modes.

Further the obtained data was compared with ab-initio calculations of antimony (Sb), which has a similar crystal structure as bismuth. Weaker spin-orbit coupling of Sb compared to Bi makes it more accesible for theory while the similarities in geometry makes a comparism reasonable. It reveals that a phonon mode measured with a nearly flat dispersion, which is usually typical for the optical branch, is an additional acoustical mode, while the estimated optical mode should occur at a higher energy.

Recent measurements performed with sample temperatures down to 115 K give more clearly resolved spectra because of the repression of multiphonon influences. Experiments using a helium beam with a larger energy up to 20 meV made it possible to reach the estimated region of the optical surface phonon branch.

- [1] P. Hofmann, Prog. Surf. Sci. 81 (2006) 191
- [2] A. Tamtögl et al., JPCM 22 (2010) 304019