Thermal diffuse scattering
in grazing incidence diffraction

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Inelastic scattering processes of hard x-ray radiation have received increasing attention in recent years. One of such inelastic decay channels is the scattering of x-rays by thermal phonons, the thermal diffuse scattering (TDS). The main features of TDS associated with Bragg diffraction have been studied in [1]. However, as a result of a sufficiently large extinction length, the surface effects were not investigated. Moreover, in most of the previous works it was assumed that the main contribution of inelastic scattering processes of x-rays is due to the scattering by the bulk acoustic modes of thermal vibrations. In a recent paper theoretically was studied the bulk and the surface excitations [2].

Using grazing incidence diffraction (GID) technique an experiment was carried out at the beamline W1. Different behavior was found for a pure GaAs crystal and a C-doped p-GaAs wafer. The general features of the GID method for investigations of the near surface properties of solids have been described elsewhere [3]. As in ordinary GID scattering the Bragg reflection is observed corresponding to a reciprocal lattice vector $H$. At the same measurement TDS is excited also at another reciprocal lattice vector $G$. As the main reflection $H$ (2 2 0) is considered. The crystal surface was parallel to the [1 0 0]. TDS is observed near the two reciprocal-lattice points $G$ (6 2 0) and (7 1 0) separated by the phonon wave vector $q$. The simultaneous excitation of $H$ and $G+q$ requires precise energy calibration. In the described scattering geometry the incident energy is in the range of 9.5-10.5 keV. During TDS-experiment two detectors are used: a mono-energetic detector for the elastically scattered beam and an energy-dispersive detector for the inelastically scattered beam (in order to separate TDS and Compton scattering).

The left figure shows a schematic layout of the experimental setup. Here $k_0$ and $k_i = k_0 + H$ are projections of the respective wave vectors onto the crystal surface with respect to the incident and diffracted beam, respectively. $k = k_0 + G+q$ is the projection of the inelastically scattering x-rays onto the crystal surface. Both $H$ and $G$ are parallel to the surface. The reciprocal lattice vector $G$ is selected in such way that the distance from the end of this vector to the Ewald sphere with a radius $k = k_0 = k_i = k_f$ is in the order of the phonon wave vector $q$. Under these conditions multiple-wave elastic diffraction scattering does not almost occur. However, one can detect a strong one-phonon inelastic scattering in the direction of $k$. The following general case is considered: both incident and diffracted beams angles are smaller or larger than a critical angle for the total external reflection $\alpha_c$. For the fixed incident angle, $\alpha_i$, one can register diffuse scattering for different angles $\alpha_{TDS}$ of the inelastically scattered beam and detect the TDS signal from different penetration depths.

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Figures: Schematic view of the TDS experiment and the inelastic scattering geometry in reciprocal space for GID conditions; TDS and D are the inelastically scattered and diffracted beam detectors, respectively (left).

Experimental curves for diffracted beam (220) and the TDS yield near reciprocal lattice vector (620) for a GaAs-wafer (top right); the same curves (bottom right) for p-GaAs (C=2e16 cm⁻³).

References