ESRF	**Experiment title:** Surface and bulk contributions to X-ray thermal diffuse scattering	**Experiment number:** ME-349
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Shifts: 12	**Local contact(s):** T.H. Metzger, A. Mazuelas	

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Report:

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 have been studied using conventional Bragg scattering technique in [1]. Due to the large extinction length, the surface effects could not be resolved. 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. The contriburion of the surface excitations to the total TDS signal were studied in a recent papers [2,3]. It was predicted that in the long-wavelength limit near the surface the contribution of the surface excitations to TDS becomes comparable to and can even exceed the bulk contribution.

The aim of the present experiment was the confirmation of these theoretic predictions by the measurement of the surface and bulk thermal excitations using x-ray grazing incidence diffraction (GID) technique. The general features of the GID method for investigations of the near surface properties of solids have been described elsewhere [4]. X-ray GID geometry is capable to obtain information about surface and bulk thermal phonons. Its particular depth sensitivity provides information about the thermal excitations in different depths below the sample surface.

The experiment was carried out at the beamline ID1 at ESRF. The beamline is especially designed to achieve a large tunable energy-range, good energy resolution and signal-to-noise ratio. The sample was a GaAs wafer with a high polished (0 0 1) surface. In order to detect TDS the reflection H=(2 2 0) was excited as a main reflection, measured for the different angles of incidence α_i. At the same time, TDS was observed in the vicinity either G=(10 2 0) or G=(12 0 0) reciprocal-lattice points. This correspond approximately to an excited dynamical three-beam case. For the diffraction vectors $\boldsymbol{H}$(2 2 0) and $\boldsymbol{G}$ =(10 2 0) the exact triple-point appers at an energy of 15.81 keV. In this case, both vectors, $\boldsymbol{H}$ and $\boldsymbol{G}$ lie on the same Ewald sphere. A slight increase of the energy of the incident beam results in a small distance between $\boldsymbol{G}$ and the Ewald sphere. This small distance corresponds to the range of accessable phonon vectors $\boldsymbol{q}$. In order to obtain $\boldsymbol{q}/\boldsymbol{G}$ ratio similar to [5] we used a photon nergy of 15.9 keV in further measurements.

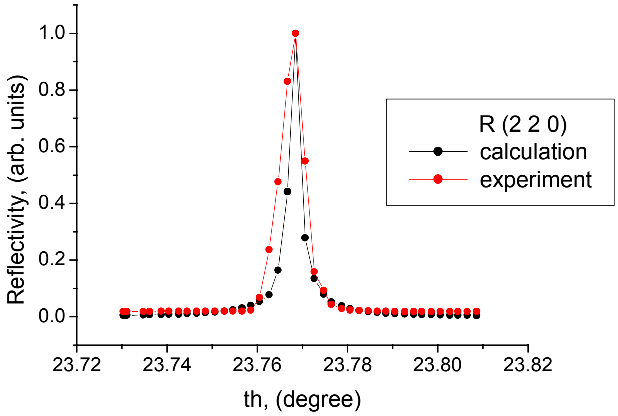

Fig. 1a experimental and calculated curves of the main reflection H (2 2 0) for the α_i =0.17 °

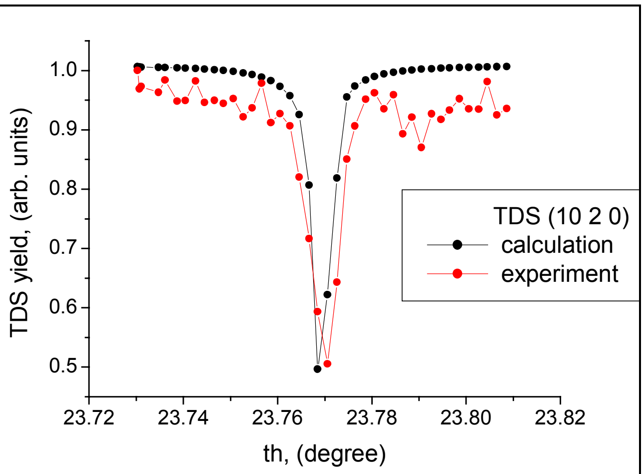

Fig. 1b the same curves for TDS yield measured near reciprocal lattice point *G* (10 2 0)

During the TDS-experiment two detectors were used: a scintillation detector for the elastically scattered beam at (2 2 0) Bragg position and a position sensitive detector (PSD) for the inelastically scattered beam near the (10 2 0) or (12 0 0) reflections. The advantage of PSD was the possibility to detect TDS signals depths for the each fixed α_i. Fig. 1 shows simultaneously measured elastic scattering of the (220) main reflection (Fig. 1a) and the TDS yield (Fig. 1b) near (10 2 0) reflection, together with the theoretic fit. As a main result, the TDS yield shows a dip in the intensity, where the elastic scattering has maximum. Following the predictions in [2,3] this dip is due to bulk thermal excitations. Fig. 2 presents the variation of the TDS signal (as in Fig. 1b) as a function of the incident angle at the main reflection. As shown the depth of the dip varies with the α_i. The angle α_i =0.17 degree corresponds to the penetration depth of about d =50 nm. At the critical angle α_c =0.16 degree d ≈25 nm and for the α_i =0.12 degree we register only a weak surface signal at the penetration depth d =7 nm.

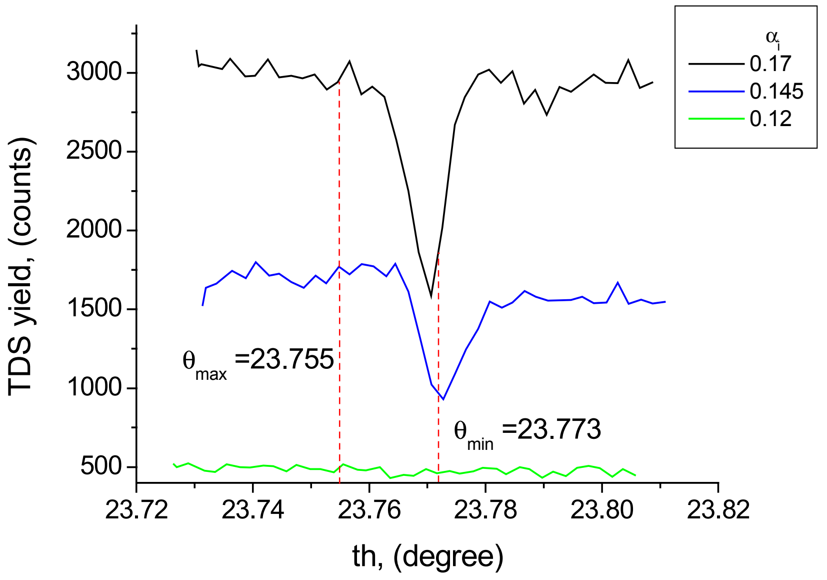

Fig. 2 experimental curves of the TDS yield as a function of the deviation from exact Bragg position for the different angle of incidence

It is evident, that the contribution of the surface TDS to the total TDS yield has to increase with decreasing of α_i. The strong surface contribution is expected close to the critical angle α_c =0.16 degree (penetration depths from 10 to 30 nm). In order to qualify this effect we selected two θ-angles, θ_{min} and θ_{max} (Fig. 2), and calculated the TDS intensity ratio $I(\theta_{max})/ I(\theta_{min})$ as a function of α_i.

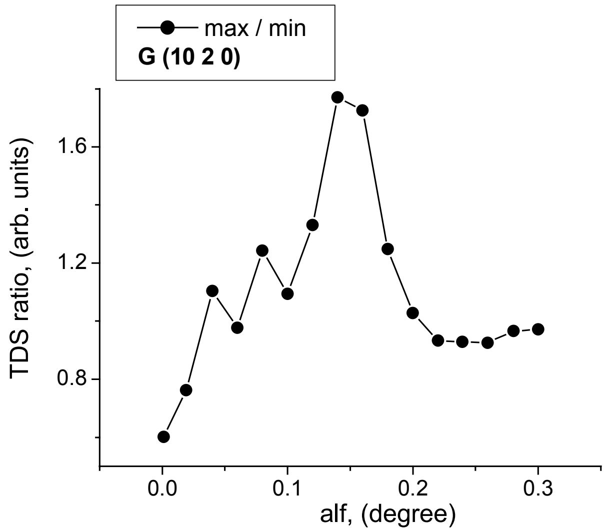

Fig. 3 TDS ratio as a function of the angle of incidence near reciprocal lattice point (10 2 0)

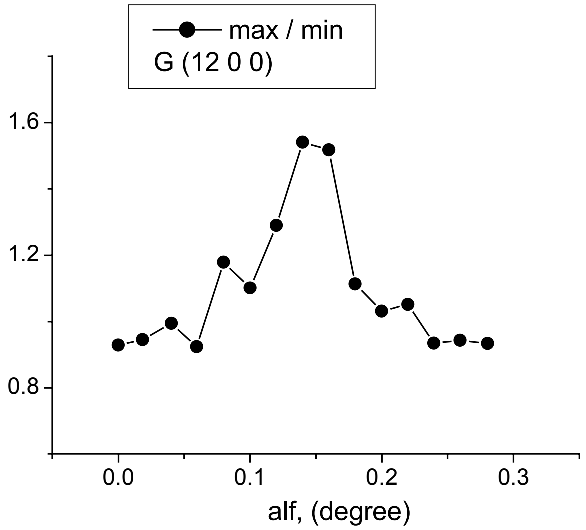

Fig. 3b the same near reciprocal lattice point (12 0 0)

This is shown in Fig.3a for *G*=(10 2 0) and in Fig. 3b for *G*=(12 0 0) reciprocal-lattice points. Both graphs display a maximum of the TDS ratio at $\alpha_i \approx \alpha_c$. The maximum correspond to the maximum yiels of the surface phonos. This is in a good agreement with the theoretical predictions, derived from Green's function approach [3]. The presented experiment is the first experimental proof of the surface contribution to the TDS.

Literature:

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