ESRF	**Experiment title:** Thermal Motion Induced Scattering from CdSe	**Experiment number**: 28-01 853
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Report 28-01 853

The aim of the current project is to develop our understanding of the physical processes involved in the excitation of forbidden reflections in Resonant X-ray Scattering (RXS). One such process is Thermal Motion Induced Resonant Scattering (TMI). Excitation arises due to dynamic displacement of the resonant atoms from the highly symmetric sites.

Until now TMI has only been observed in three crystals, namely Ge [i,ii], ZnO [iii], and GaN [iv]. The latter two systems exhibit similar TMI signatures, contrasting with that of Ge. This is perhaps not surprising as Zn/Ga and N/O are adjacent in the periodic table, and the compounds have similar electronic structure and lattice dynamics. CdSe, on the other hand, is isostructural with these compounds but contains elements of very different mass. Moreover, both elements have accessible absorption edges in the X-ray regime resonances. This allows a direct comparison of the TMI signature for each element. To this end TMI measurements were attempted at the Cd L1, L2 and L3 edges. We also aimed to measure Se K edge but with time constraints and experimental difficulties, this was not possible.

The (2 -1 1) reflection was chosen because, while forbidden by the space group symmetry, it can be observed due to the anisotropy of the atomic orbitals. Fig. 1 shows the calculated relative scattering intensity for the (2 -1 1) reflection as a function of azimuth defined with respect to the (0 0 1) azimuthal reference. The scattering cross-section exhibits a strong azimuthal dependence which introduces a constraint in the azimuthal selection which can lead to problems with multiple scattering.

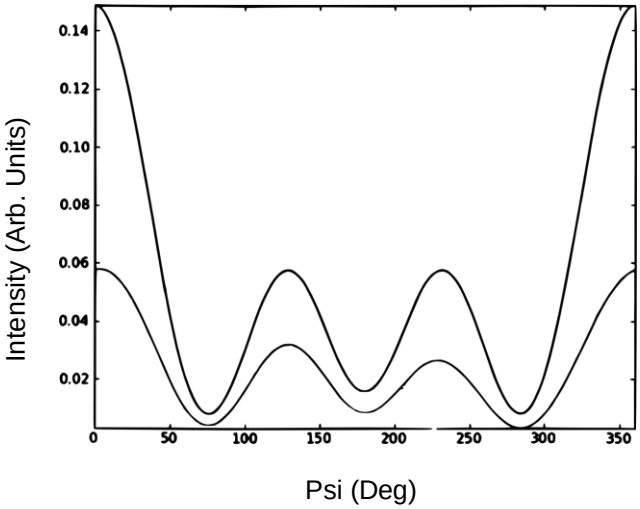


Fig. 1. Simulated azimuthal dependence of the scattering cross-section.

Multiple scattering can usually be avoided by either changing the incident energy or changing the azimuthal angle (fig. 2). However, as the TMI measurements must be carried out at resonance, and in an azimuthal region were the scattering intensity is strong, the conditions for extracting the TMI signature are less than optimum.

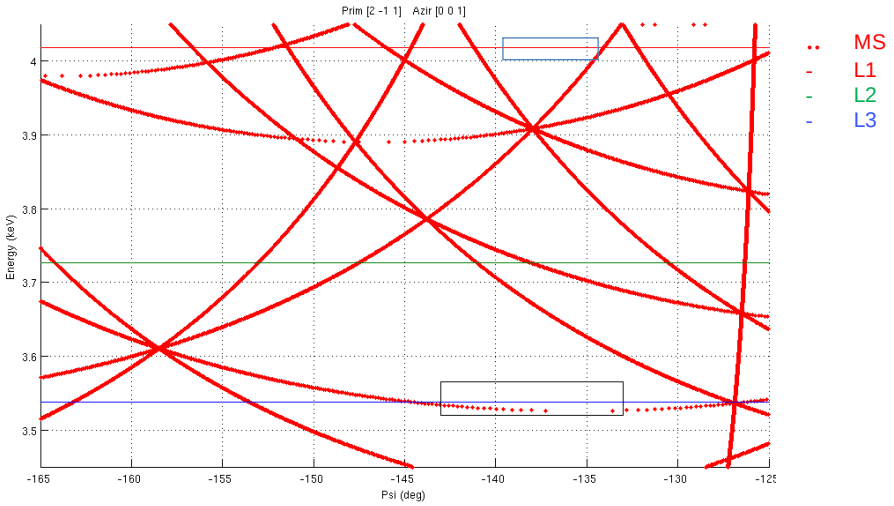


Fig. 2. Simulated multiple scattering positions as a function of energy and azimuthal angle. The black and blue rectangles represents the regions where the L3 and L1 TMI signatures were measured, respectively.

There is a region around -160° which is clear of multiple scattering at the L3 edge; unfortunately the scattering cross-section in this region is at a minimum. The L3 measurements were carried out in the region represented by the black rectangle in fig. 2. In order to separate the E1-E2 signal from the TMI signal, the energy scans on the appropriate reflections are carried out over a range of temperatures, 100 K – 600 K in this case. The following plots show the TMI scans at two azimuths; -143º and -133º.

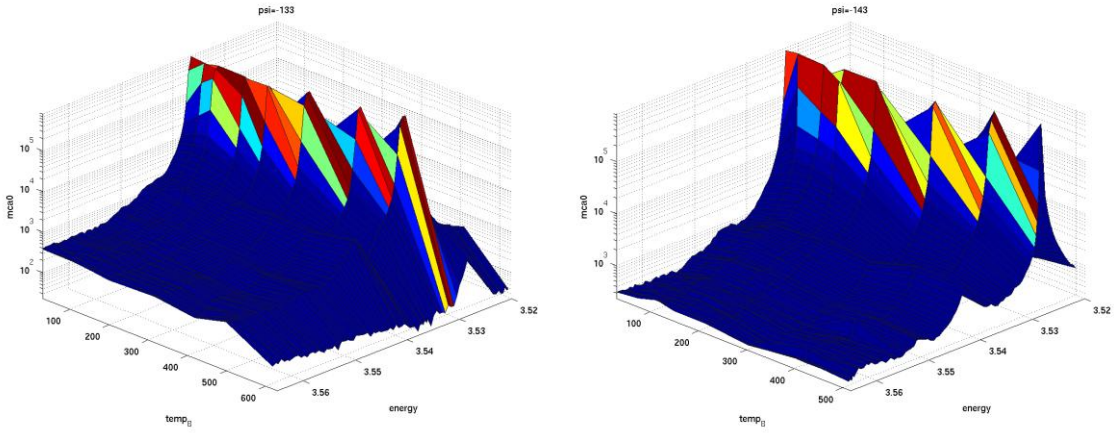
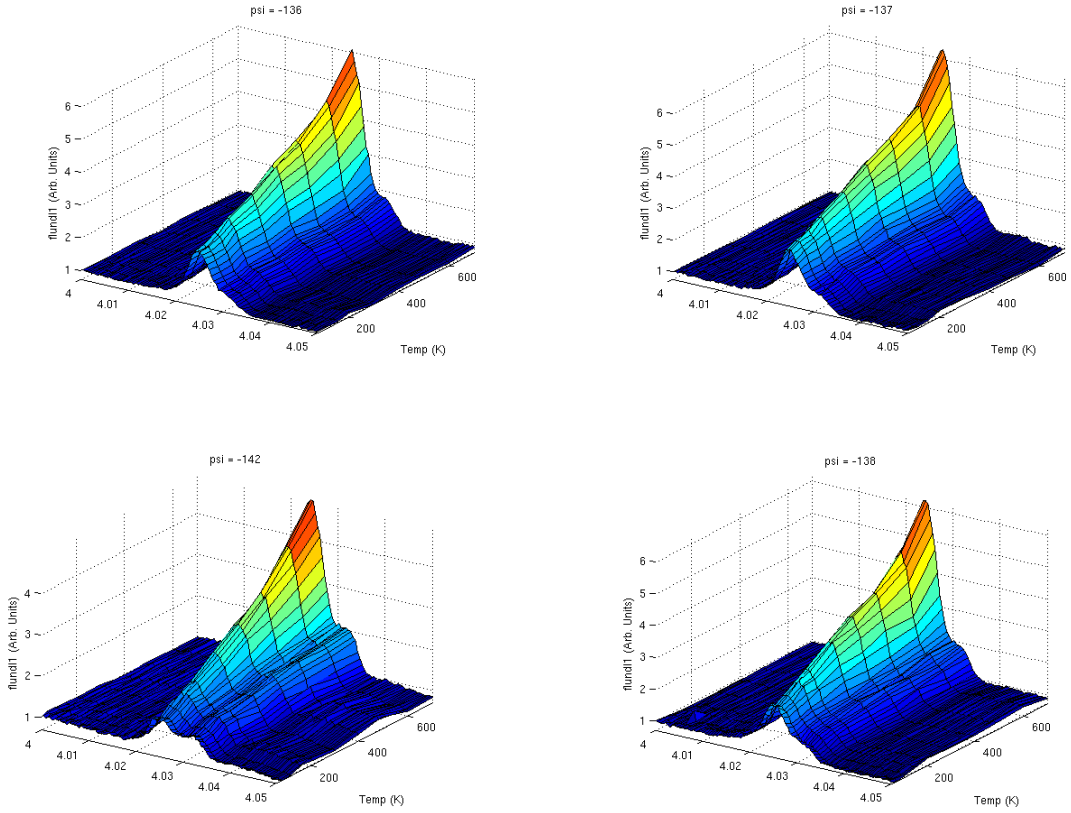


Fig. 3. TMI scans over a temperature range of 100 K – 600 K and energy range of 3.52 to 3.565 keV (Cd L3 edge) for azimuths ranging from -143º to -133º. Both plots are dominated with multiple scattering.

The E1-E2 and TMI components of the (2 -1 1) reflection are obscured by the tail of the multiple scattering peak which is further complicated by the fact that the MS peak shifts with temperature. Despite this complication, two peaks aside from the MS peak, are observable. However, both appear to show the same temperature dependence.

We had better success with the L1 edge. Interestingly, unlike the ZnO and GaN, the CdSe exhibits no temperature dependent contribution which suggests the TMI signature is more electronically dependent than structurally dependent.



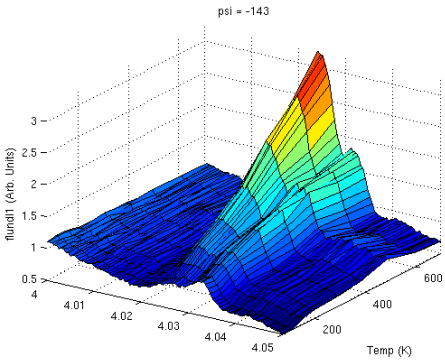


Fig. 4. TMI scans over a temperature range of 100 K – 600 K and energy range of 4 to4.05 keV (CdSe L1 edge) for azimuths ranging from -136º to -143º.

We also attempted to measure at the L2 edge, however the (2 -1 1) reflection was too week to be useful. Finally, as the Se K edge occurs at 12.6578 keV, the (2 -1 1) reflection is crowded with multiple scattering and would be unlikely to provide anything useful. Data analysis is on-going but severely hampered by these multiple scattering contributions.

Finally, we note that these measurements were carried out in preference to the original plan, to look at similar effects in KDP. This is because preliminary studies on the latter suggested that severe radiation damage in these materials made high quality data collection highly unlikely.

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i J. Kokubun, M. Kanasawa, K. Ishida, V.E. Dmitrienko, *Phys. Rev. B* **64**, 073203 (2001).
ii A. Kirfel, J. Grybos, V.E. Dmitrienko, *Phys. Rev. B* **66**, 165202 (2002).
iii S.P. Collins, D. Laundry, V.E. Dmitrienko, D. Mannix, P. Thompson, *Phys. Rev. B* **68**, 064110 (2003).
iv Unpublished data taken at XMaS, ESRF-XMaS experimental report **28-01-853**.