	Experiment title: Pressure-dependent nuclear inelastic and nuclear forward scattering in Ge2Sb2Te5	**Experiment number**: HS4778
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Report:

During the beam time allocated for proposal HS 4778 ^{121}Sb and ^{125}Te nuclear inelastic scattering (NIS) at an energy of 37.1 keV and 35.5 keV, respectively, was carried out in the phase change materials Sb_2Te_3 and $GeSb_2Te_4$ at pressures up to 76 GPa. This experiment was the first demonstration of the feasibility of high pressure ^{121}Sb and ^{125}Te nuclear inelastic scattering. The experimental setup is therefore described in more detail.

The experimental setup consisted of a medium resolution monochromator, a high resolution sapphire backscattering monochromator, a 16 element detector array of silicon avalanche photodiodes, a pair of two silicon avalanche photodiodes, a KB x-ray focusing optic, a diamond anvil pressure cell and a MAR image plate detector, which was only used for XRD measurements. The backscattering monochromator is necessary in order to achieve the required energy resolution of a few ~meV.

The high pressure cells used in this experiment are especially desgined to fulfill the requirement that the direct beam remains undeflected and bypasses the cell below while the backscattered beam passes through the cell along the centre axis. In the first attempt without the KB x-ray optic it was not possible to detect any resonant signal due to a large beam size of 0.56 and 0.35 mm in vertical and horizontal direction, respectively. It was therefore necessary to use the KB x-ray optic in order to focus the backscattered beam on the small sample volume inside the pressure cell. However, the geometry of the experimental setup did not allow for installing the KB x-ray optic in the backscattered beam without blocking the direct beam. This problem was solved by rotating the pressure cell by 90° so that the beam was perpendicular to the centre axis and by aligning the backscattering monochromator for beam deflection in the horizonzal instead of the usual vertical direction. In this configuration it was possible to measure the ^{125}Te NIS signal with a beam size of 0.024 and 0.023 mm in vertical and horizontal direction, respectively. However, due to the large horizontal beam divergence the energy resolution was about ~4 meV. Mechanical slits were used to decrease the beam divergence of the direct beam which improved the energy resolution to about ~1.9 meV. For the XRD measurements the sample and the MAR image plate were moved into the direct beam. A cerium dioxide sample was used as a reference.

^{125}Te NIS was measured in isotopically enriched $GeSb_2{}^{125}Te_4$ powder in the cubic phase at pressures of 10.6 and 16.2 GPa and in $Sb_2{}^{125}Te_3$ powder at pressures of 14.8 and 76.2 GPa. In addition, ^{121}Sb NIS was measured in $Sb_2{}^{125}Te_3$ at a pressure of 76.2 GPa. All measurements were performed at room temperature. The applied pressure was measured with the ruby fluorescence method and with the XRD spectrum of KCl which was added to the pressure cells as a further reference. Representative raw ^{125}Te NIS spectra including the instrumental resolution functions for $GeSb_2{}^{125}Te_4$ and $Sb_2{}^{125}Te_3$ are shown in Figure 1 - 3. Since the measurements were performed at room temperature strong multiphonon contributions can be observed. These correspond to a small Lamb-Mössbauer-factor f_{LM}, e.g. for ^{125}Te in $GeSb_2{}^{125}Te_4$ at 16.2 GPa f_{LM} = 0.04(2), and prevent the extraction of the density of phonon states (DPS) for the low pressure measurements.

However, the ^{125}Te spectrum of $Sb_2{}^{125}Te_3$ at 76.2 GPa clearly reveals one phonon contributions and it is possible to extract the ^{125}Te element specific DPS, see Figure 4. The Lamb-Mössbauer-factor is determined to be 0.40(1).

In summary, the feasibility of high pressure ^{125}Te and ^{121}Sb NIS was demonstrated. Although the measurements were performed at room temperature it is possible to extract the DPS provided the applied pressure is sufficiently high. The possibility of simultaneously cooling the samples should be pursued for future experiments.

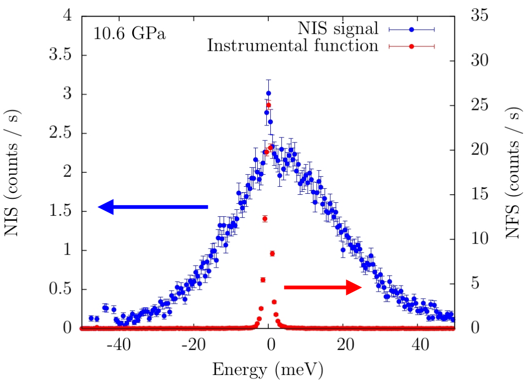

Fig.1: NIS signal and instrumental function of ^{125}Te in $GeSb_2Te_4$ at 10.6 GPa.

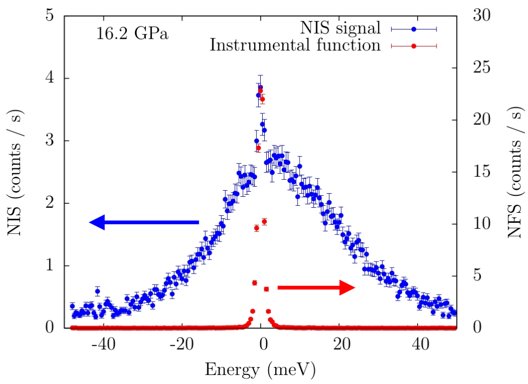

Fig.2: NIS signal and instrumental function of ^{125}Te in $GeSb_2Te_4$ at 16.2 GPa.

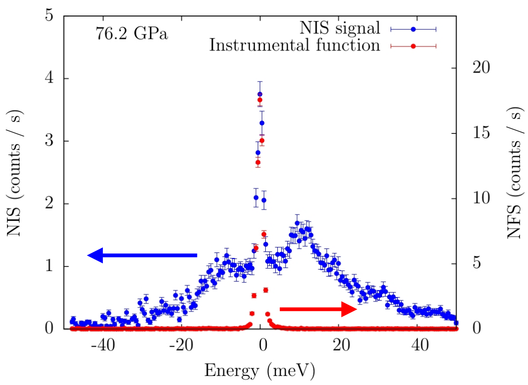

Fig.3: NIS signal and instrumental function of ^{125}Te in $Sb_2{}^{125}Te_3$ at 76.2 GPa.

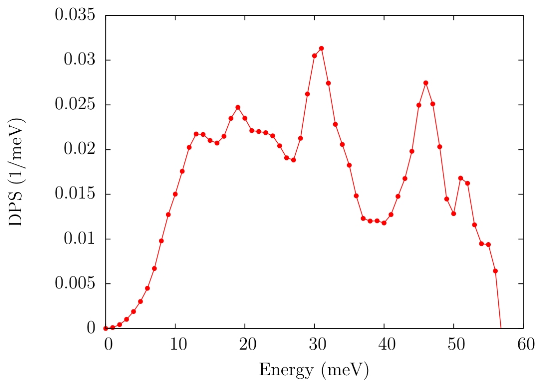

Fig.4: ^{125}Te element specific DPS in $Sb_2{}^{125}Te_3$ at 76.2 GPa.