	Experiment title:	Experiment number:
ESRF	Softening upon crystallization and anharmonicity in the $SnSb_2Te_4$ phase change material	HS-4369
Beamline: ID18	**Date of experiment:** from:05/05/2011 to: 10/05/2011	**Date of report:** 10/10/2011
Shifts: 18	**Local contact(s):** Dr. Aleksander Chumakov (email: chumakov@esrf.fr)	*Received at ESRF:*

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Report:

In the allocated beamtime we investigated the lattice dynamics of the phase change material $SnSb_2Te_4$ by means of nuclear inelastic scattering (NIS) using the sapphire backscattering monchromator [1] providing instrumental resolution of ~1meV at ID18. The measurements were performed on the three Mößbauer active isotopes: ^{119}Sn, ^{121}Sb and ^{125}Te in the amorphous, cubic and hexagonal phase. Typical raw spectra measured at 20 K on the hexagonal phase in all three isotopes are shown in Fig. 1.

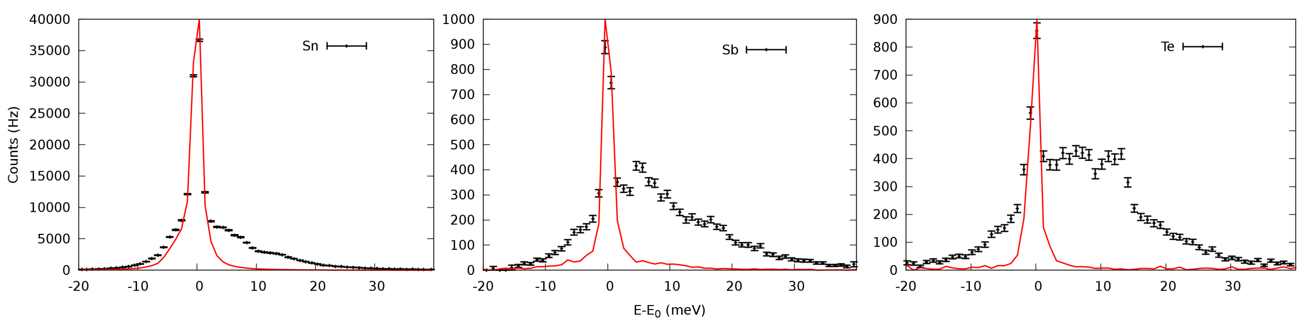

Fig. 1: NIS spectra of hexagonal $SnSb_2Te_4$ measured at 20K on ^{119}Sn, ^{121}Sb and ^{125}Te. Inleastic spectrum (black points) and instrumental function (red line).

From the evaluation of the raw spectra, the density of phonon states (DPS, g(E)) was extracted for the three isotopes ^{119}Sn, ^{121}Sb and ^{125}Te in all available phases using the program DOS [2] and given in Fig. 2. A hardening of the acoustic modes upon crystallization, below 5meV, is observed. At the same time, a related softening which is expressed by the shift of the high energy optical modes for Sb and Te is also observed. Similar effects have been measured for the isoelectronic material $GeSb_2Te_4$ [3]. Ge NIS is not feasible. The additional information obtained in this investigation was the contribution of Sn which at the same time gives us the opportunity to better understand the Ge contribution in the isoelectronic $GeSb_2Te_4$ phase change compound.

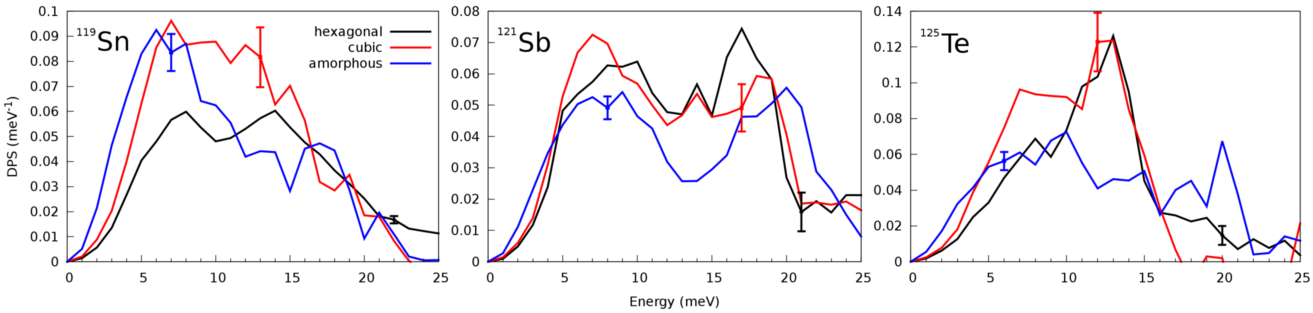

Figure 2: The extracted density of phonon states using the DOS [2] for the isotopes ^{119}Sn, ^{121}Sb and ^{125}Te in hexagonal, cubic and amorphous phase.

The mean force constants, second moment of the density of phonon states, and Debye energy, E_D, obtained from the low energy limit as $\frac{3}{\boldsymbol{E}_D} = \lim_{E\to 0} \sqrt[3]{\boldsymbol{E}^2 / \boldsymbol{g}(\boldsymbol{E})}$ was also extracted from the density of phonon states and included in Table 1.

	Force constant, N/m			
Phase	Sn	Sb	Te	**E_D, meV**
Amorphous	63	94	79	10
Cubic	65	74	66	14
Hexagonal	64	76	70	13

Table 1: The extracted thermodynamical parameters from the measured density of phonon states, the mean force constants and the speed of sound u_s

Although a systematic hardening of the atomic bonds is indicated in the extracted speed of sound for all three phases, the opposite is observed in the extracted mean force constants of tellurium and antimony atoms. Exception is the extracted mean force constant of tin which is approximately the same for all three states. This peculiarity is now being examined

In summary, we have proven feasibility of measuring NIS on all three different Mößbauer active isotopes: ^{119}Sn, ^{121}Sb and ^{125}Te of $SnSb_2Te_4$ during experiment HS-4369 using a backscattering monochromator [1].

References

[1] I. Sergueev *et al.*, *J. Synchrotron Rad.* **18**, 802 (2011).
[2] V. G. Kohn and A. I. Chumakov, *Hyperfine Interact.* **125**, 205 (2000).
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