ESRF	**Experiment title:** Unusual doping effects on lattice thermal conductivity in thermoelectric Mo3(Sb,Te)7	**Experiment number:** HC-1085
Beamline: ID18	**Date of experiment:** from: 27.08.13 / 13.09.13 to: 30.08.13/16.09.13	**Date of report:** 25.02.2014
Shifts: 18	**Local contact(s):** Dimitrios Bessas	*Received at ESRF:*

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Report:

Within the beam time allocated for proposal HC-1085 the lattice dynamics in different compounds of the $Mo_3Sb_{7-x}Te_x$ series were investigated using nuclear inelastic scattering (NIS) by both the ^{121}Sb and ^{125}Te Mössbauer resonance.

The carrier concentration of the Mo_3Sb_7 compound can be effectively optimized by Te substitution on the Sb site for thermoelectric purposes. However, beside its effect on carrier concentration the Te substitution also results in an unexpected increase of lattice thermal conductivity [1]. Thus, this investigation of lattice dynamics using NIS aimed at a microscopic understanding of this unusual effect of doping.

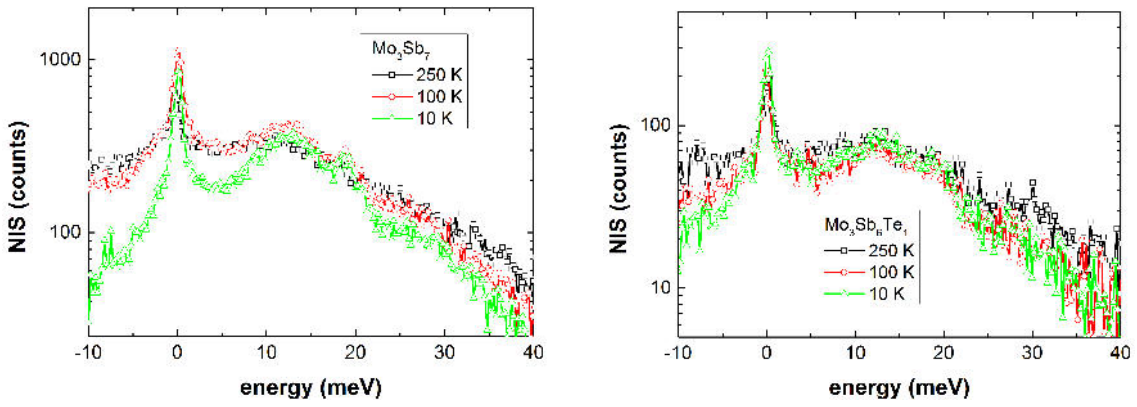

*Fig. 1: Representative ^{121}Sb specific NIS spectra for Mo_3Sb_7 (**left**) and $Mo_3Sb_6Te_1$ (**right**) obtained at different temperature.*

In Fig. 1 representative NIS spectra of Mo_3Sb_7 and $Mo_3Sb_6Te_1$ obtained using the ^{121}Sb resonance are shown. They are predominantly characterized by strong phonon contributions between 10 and 25 meV. It also apparent that multiphonon contributions significantly increase at higher temperatures which complicates density of phonon states (DPS) extraction using the Fourier-Log decomposition procedure [2]. However, both for ^{121}Sb and ^{125}Te NIS measurements an instrumental resolution (full width at half maximum) of about 1.1 meV could be achieved.

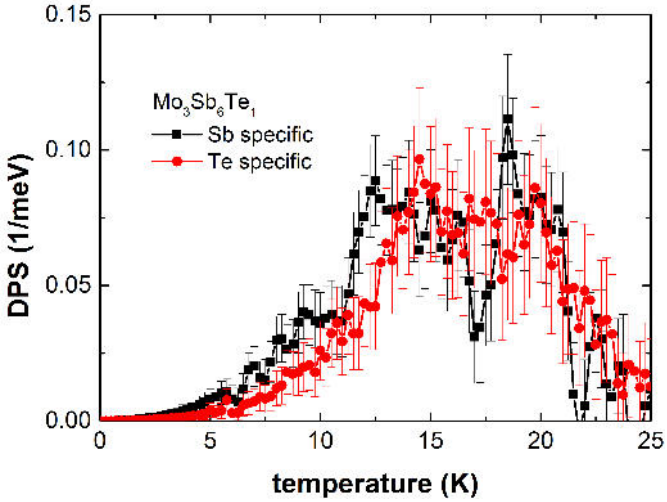

Fig. 2: ^{121}Sb and ^{125}Te specific density of phonon states (DPS) in $Mo_3Sb_6Te_1$ at 10 K.

An example for the element specific density of phonon states is shown in Figure 2 for $Mo_3Sb_6Te_1$ at 10 K. Both DPS exhibit phonon modes up to about 25 meV and, within the error bar, mostly differ in the low energy region below 12.5 meV.

All in all, three compounds with x=0, 1, 1.8 could be investigated using NIS by both resonances aforementioned at three different temperatures, i.e. at 10, 100 and 250 K. A more detailed analysis of force constants [3], speed of sound values as well as the extraction of DPS at high temperatures will allow further insight in the scientific case discussd above.

References

[1] X. Shi et al., Energy Environ. Sci. 4 (2011) 4086.
[2] V. G. Kohn and A. I. Chumakov, Hyperfine Interact. 125 (2000) 205.
[3] M. Hu et al., Phys. Rev. B 87 (2013) 064301.