ESRF	**Experiment title:** Determination of the Sb partial density of states in skutterudites using nuclear inelastic scattering on ^{121}Sb at 37.13 keV	**Experiment number:** HS-2928
Beamline: ID18	**Date of Experiment:** from: 06/02/2006 to: 14/02/2006	**Date of Report:** January 17, 2007
Shifts: 18	**Local contact(s):** Dr. Ilia Sergueev	*Received at ESRF:*

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Report:

The observation of nuclear resonant scattering from ^{121}Sb at the 37.13 keV [1] in a recent experiment (MI-710) provided a route by which nuclear inelastic measurements may be obtained for this nuclide. For details see [1] and references given there. During the experiment HS-2928 nuclear inelastic scattering (NIS) from antimony compounds has been observed. To our knowledge this have been the first dynamical studies using this technique for this nuclide and at a nuclear transition energy above 30 keV in general. High resolution monochromatization in the meV range, required two resolve the phonon energy spectra, was achieved by using a Bragg backscattering monochromator [1,2] consisting of a sapphire (α-Al_2O_3) crystal located in a temperature controlled liquid N_2 flux cryostat with mK stability. The monochromator is an improved rebuilt version of the monochromator used for the studies in the experiment MI-710. The photon energy of the reflected radiation is modulated by changing the temperature of the sapphire crystal both above and below 146.54 K, the temperature corresponding to the Mössbauer resonance energy E_0=37.1298(2) keV; the variation in the photon energy at this temperature is 59.6 meV/K.

The samples were an unfilled and a filled skutterudite, namely $CoSb_3$ and $EuFe_4Sb_{12}$. Their comparison is of high interest for the understanding of the dynamics in filled skutterudites. The latter are broadly studied due to their interesting thermoelectric properties. The so called figure of merit, which is proportional to its electronic conductivity and inversely proportional to its thermal conductivity, of these materials is high, which makes them excellent candidates for this application.

The absorbers were in the form of polycrystalline powder mixed with boron nitride and placed in a closed cycle cryostat at an estimated temperature of 25 K.

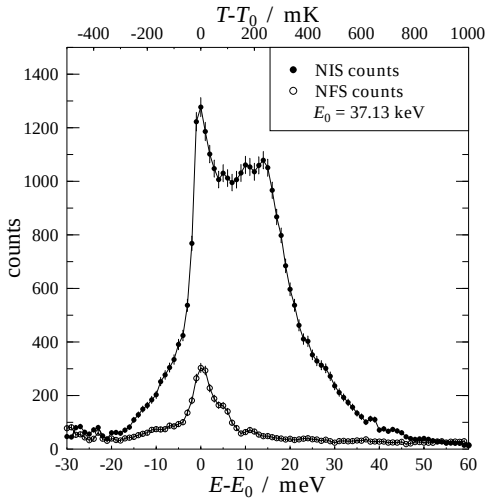

Fig. 1: Temperature/energy dependence of the nuclear forward, open symbols, and nuclear inelastic, closed symbols, scattered intensity from $EuFe_4Sb_{12}$. The lines are a guide for the eye.

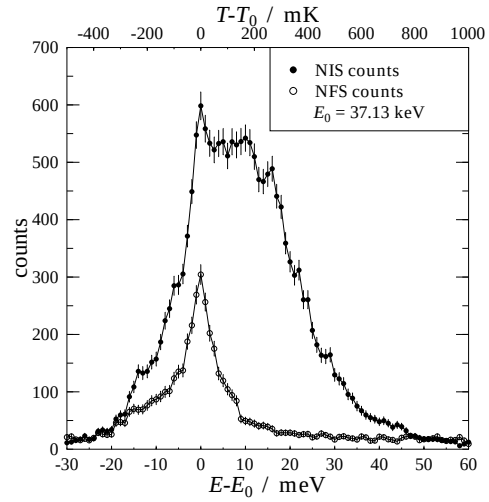

Fig. 2: Temperature/energy dependence of the nuclear forward, open symbols, and nuclear inelastic, closed symbols, scattered intensity from $CoSb_3$. The lines are a guide for the eye.

In figure 1 and figure 2 energy spectra of the nuclear forward scattered (NFS) and the nuclear inelastic scattered intensity (the phonon energy spectra plus a contribution of the elastic peak around E_0) of $CoSb_3$ and $EuFe_4Sb_{12}$ are shown. The instrumental resoluton is given by the width of the elastic nuclear forward signal and was about 6 meV at best.
In the subsequent experiment HS3041 at ID22 the data statistic has been improved and a resolution of 4.5 meV was achieved. As a result the antimony partial vibrational density of states in $CoSb_3$ and $EuFe_4Sb_{12}$ was obtained. These results together with earlier NFS studies on Fe and Eu lead to a complete experimental determination of the partial vibtational DOS associated with all the elements in $EuFe_4Sb_{12}$ and provided new insight in the dynamics and especially in the hybridization mechanism between the rattler and the surrounding cage in filled skutterudites. The results are presented and discussed including a comparison of the experimental data to theoretical calculations in a paper to be published soon (submitted to Physical Review Letters).

References

[1] H.-C. Wille, Yu. V. Shvyd'ko, E. E. Alp, H. D. Rüter, O. Leupold, I. Sergueev, R. Rüffer, A. Barla, J. P. Sanchez , Europhys. Lett., 74, no.1 (170)