Local Vibrational Modes in $EuFe_4Sb_{12}$ and $Ni_{0.49}Fe_{0.01}Al_{0.50}$ Alloy

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Nuclear resonance scattering offers the possibility of determining local electronic, magnetic, structural or dynamic properties. Herein we report on studies of the local vibrational density of phonon states (VDOS) in the filled skutterudite, $EuFe_4Sb_{12}$, and in the the $Ni_{0.49}Fe_{0.01}Al_{0.50}$ alloy by applying the nuclear inelastic scattering (NIS) technique. Experiments were done at the nuclear resonance beamlines ID18 and ID22N at the ESRF.
The filled skutterudites RM_4Sb_{12} (where R = rare earth, and M = Fe or Co) exhibit promising thermoelectric properties, which are partly ascribed to the "rattling" rare earth atom in a cage formed by the M_4Sb_{12} lattice. Our NIS data obtained on ^{151}Eu in $EuFe_4Sb_{12}$ reveal a pronounced peak at ca. 7 meV, a low energy peak which is associated with the Einstein oscillator behavior of the Eu, see Figure 1. In contrast the ^{57}Fe VDOS obtained on the same sample does not exhibit any low energy peaks.

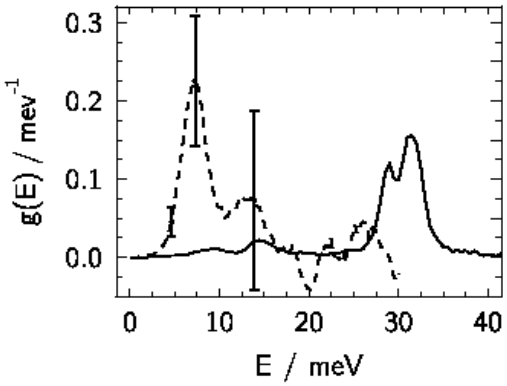

Figure 1: VDOS in $EuFe_4Sb_{12}$; full line: ^{57}Fe, dashed line: ^{151}Eu normalized partial density of states.

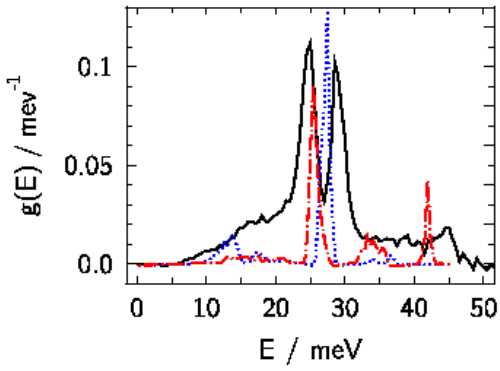

Figure 2: full line: VDOS of ^{57}Fe in an alloy of $Ni_{0.49}Fe_{0.01}Al_{0.50}$; dotted line: calculations for Fe on the Al site, dash-dotted line: calculations for Fe on the Ni site.

For diluted Fe atoms in a NiAl alloy, *ab initio* calculations have predicted a localized vibrational mode at about 26meV. We measured the ^{57}Fe partial VDOS of a $Ni_{0.49}{}^{57}Fe_{0.01}Al_{0.50}$ alloy with an energy resolution of about 0.5meV. Our results show (cf. Figure 2) two peaks at ca. 26meV. This can be interpreted as Fe substituting both Ni and Al, the latter giving rise to a localized mode at slightly higher energy than for Fe on the Ni site as confirmed by *ab initio* calculations also shown in Figure 2.