ESRF	**Experiment title:** Study of Iron partial density of phonon states in the strongly correlated semiconductor FeSi	**Experiment number**: HS-4635
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Report:

FeSi is a strongly correlated semiconductor where the gap ~70-100 meV in the electronic density of states (DOS) develops below T~200K along with the formation of the non-magnetic ground state [1,2]. The physical mechanism responsible for the temperature evolution of the electronic spectrum is not yet fully understood, and is currently the subject of intensive studies. The theoretical approaches to this problem are mostly related to the electron subsystem, but one cannot disregard a possible interplay with lattice vibrations. For instance, recently it was suggested [3] that the closing of the gap in FeSi upon the increase of the temperature could be the result of the thermal disorder affecting the electronic DOS via the electron-phonon interaction.

In the present experiment we have studied the temperature evolution of the partial density of vibrational states (PDVS) of iron ions by means of the *nuclear inelastic scattering*. The experiment has been performed at the beam-line ID18 using high-quality single phase powder sample of ^{57}FeSi (94.5% of ^{57}Fe isotope enrichment). The spectra have been recorded with energy resolution of ~1.5 meV at 7 temperature points in the range 46 – 297 K: 46K, 103K, 153K, 180K, 205K, 251K and 297 K. The Fe-PDVS has been derived from the experimental spectra using the procedure of the double Fourier transform [4].

The phonon energies were found to demonstrate considerable temperature dependence. Partly the energy renormalization is clearly driven just by the thermal expansion of the lattice. The Grüneisen parameters in FeSi are different for different phonon modes. Therefore it is not easy to separate the trivial effect due to thermal expansion from that possibly related to the evolution of the electronic and/or magnetic properties. However, one can expect that these "non-trivial" effects should be more evident after any physically reasonable scaling. One of the natural ways for scaling of the PDVS is the scaling according to the temperature variation of the Debye energy.

The Debye energy E_D has been determined from the low-energy part of the PDVS according to the formula:

$$E_D = \left[\frac{m_{Fe}}{\langle m \rangle} \frac{3}{\lim_{E \to 0} \left(g_{Fe}(E)/E^2 \right)} \right]^{\frac{1}{3}}$$

where m_{Fe} – atomic mass of Fe, <m> - the average atomic mass in FeSi, $g_{Fe}(E)$ – iron PDVS. PDVS energy scale has been corrected so that the Debye energy would be temperature-independent. PDVS amplitude was then scaled to keep the integral under the curve equal to unity. The scaled PDVS for two limiting temperatures (46K and 297K) are shown in Fig.1.

In addition to the energy renormalization PDVS clearly changes the structure in the energy range 22-27 meV. This effect is illustrated in more detail in the Inset of Fig.1. At T=46K one can clearly see the splitting of the low-energy phonon peak with well-pronounced minimum at E~23.5 meV. Taking into account the structure of the phonon dispersion curves in MeSi systems [5], we can assign this splitting to the mutual shift of the acoustic and low-energy optic phonon branches, apparently due to opening the gap in the electronic DOS.

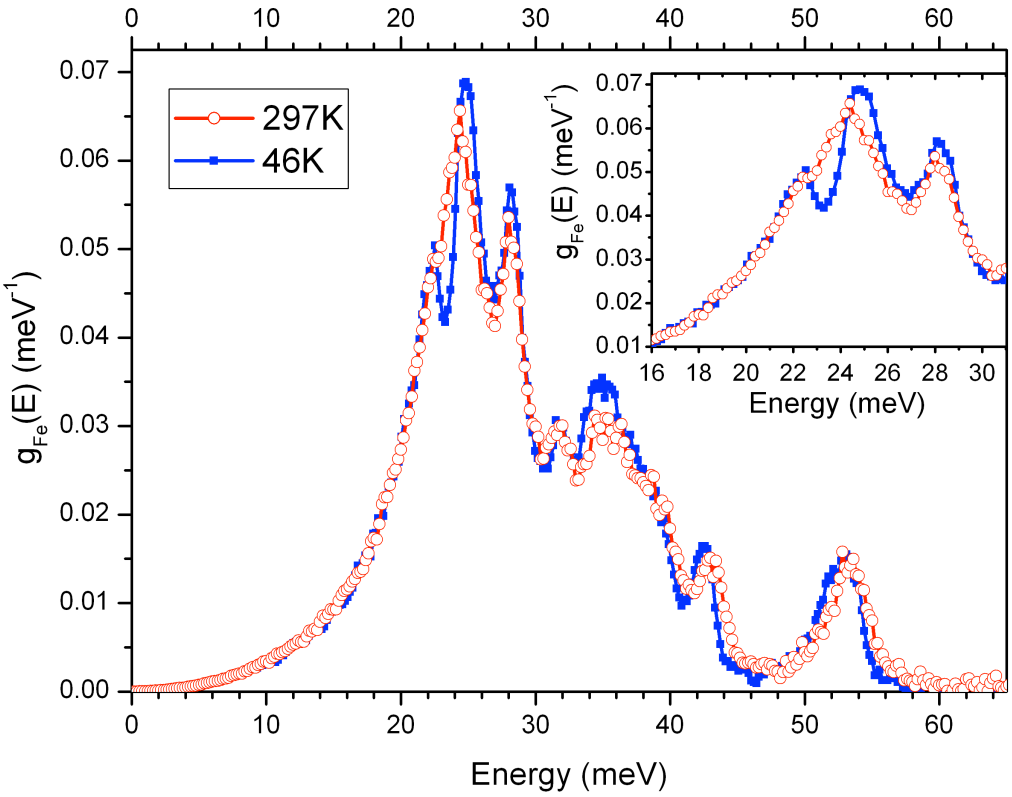

Fig.1. Partial density of vibrational states (PDVS) of iron ions at two limiting temperatures corrected for the temperature variation of Debye energy. Inset: temperature evolution of the low-energy PDVS in the enhanced scale.

References

1. Z.Schlezinger, Z.Fisk, H.-T.Zhang et.al., Phys. Rev.Lett. **71** (1993) 1748.
2. P.Nyhus, S.L.Cooper, Z.Fisk, Phys. Rev. B **51** (1995) 15626.
3. O.Delaire, K.Marty, M.B.Stone et.al., Proc. Natl. Acad. Sci. USA **108** (2011) 4725.
4. V.G.Kohn, A.I.Chumakov, Hyperfine Interactions **125** (2000) 205.
5. D.Lamago, E.S.Clementyev, A.S.Ivanov et.al., Phys.Rev.B **82** (2010) 144307.