	Experiment title: Temperatur Dependend Phonon Density of States of the Invar Alloy $Fe_{72}Pt_{28}$	**Experiment number:** HS-436
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Report:

In our experiments we investigate the balance between phase transitions and changes in the vibrational behaviour of a solid as seen in the phonon dispersion relation and the DOS. The DOS and its eventual changes with temperature gives us the entropic contribution to the Gibb's free energy, while changes with temperature in a specific part of the phonon dispersion may tell us the displacement vectors being active during the transformation. The invar alloy Fe_3Pt in it's ordered phase shows a martensitic phase transition from $L1_2$ (Cu_3Au) to a tetragonal structure at a temperature of approximately 50 K. The transition is announced by a soft mode in the $T_{[110]}$–branch of the dispersion relation. Inelastic neutron measurements[1] showed this softening at the brillon zone boundary with decreasing temperature starting already at room temperature. At the transition the phonon energy vanishes and a strong damping was observed. In our studies we want to answer the question how the phase transition and the invar property are related to this strong anharmonic effect.
Nuclear inelastic resonant absorption of synchrotron radiation[2,3,4] has developed to a new tool allowing the determination of the phonon density of states (DOS). The principle of nuclear inelastic resonant scattering with synchrotron radiation (SR) is simple. Small energy changes (meV) compared to the energy of the beam (14 keV) can be measured by tuning a high resolution monochromator around the nuclear resonance of ^{57}Fe. If the short SR-pulse excites an ^{57}Fe–nucleus in the sample, delayed fluorescence light can be detected by means of time discrimination techniques. These delayed r-quanta occur on the one hand if the SR-beam has the energy of the nuclear transition (elastic peak) and on the other hand the resonance energy can still be matched by inelastic scattering due to creation or annihilation of a phonon. For our experiment at ID18 we prepared an ordered polycrystalline Fe_3Pt foil enriched 95% in ^{57}Fe. It was mounted slightly inclined to the beam for good illumination. The detector was placed parallel to the beam and just a few millimetres apart from the sample allowing to measure the fluorescence quanta within a significant solid angle. By tuning the energy of the incident beam in the range of $\pm$ 60meV around the nuclear resonance we got the absorption spectrum (fig. 1)

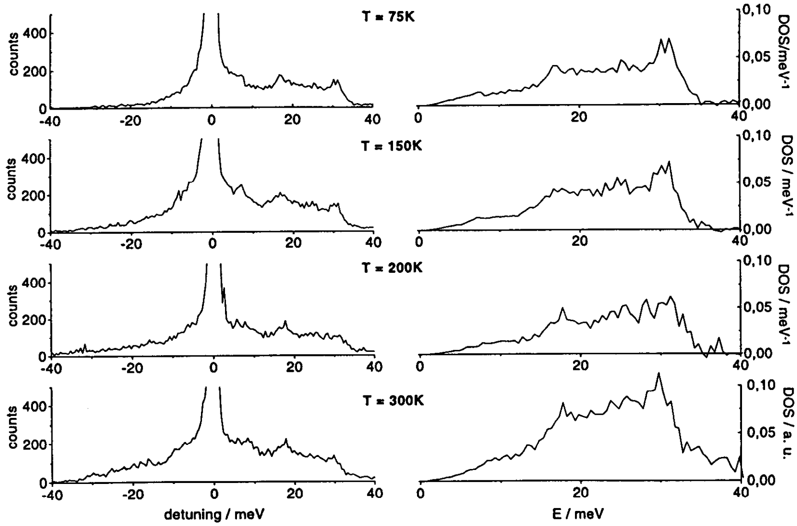

fig. 1: Phonon spectra (1) and DOS (2) of Fe_3Pt at different temperatures. The DOS at 300K is calculated ignoring multi phonon terms, as statistics was to bad for further evaluation; the peak near 1 meV is an artifact due to the subtraction of the elastic peak.

and the DOS (fig.2). The resolution of 0.8meV obtained with a highly asymmetric Si (975) double crystal monochromator[5] is to our knowledge the best value ever obtained using inelastic scattering of synchrotron radiation. It is obvious that the spectra and the DOS have a temperature dependent shape, an indication for the anharmonic behaviour. On top of the smooth intensity distribution three features may be discerned in spite of the fact, that the statistics is not yet satisfactory: The peak at 7.5 meV reflecting the soft mode in the $TA_{[110]}$ develops on cooling from from 295 K to 75 K (arrow in Fig. 2).At the lowest temperature is shows up as a kink, characteristic for the maximum in the dispersion relation[6].
Next, near 18 meV, we observe a peak corresponding to an optical phonon, found in all three high symmetry directions. Within the accuracy of the present data, this phonon shows no change with temperature, the peak remains at the same position and shows no significant broadening.
In contrast to this, the optical phonon at 30 meV shows a softening of about 10% in the temperature range investigated. This part of the DOS behaves rather normal, the frequency of the phonon decreases with increasing temperature. Also a broadening of the peak is observed, which indicates a stronger damping of those optical modes.
Finally we want to stress, that the DOS does not correspond to the data published in [6], even taking the smearing with the resolution of 0.8 meV into account. First our data reflect only the motion of the iron, the platinum is contributing only via second order effects. So part of the difference may be found in this fact. Second, calculating the DOS in Born-von Karman approximation as done in [6], implicitly assumes at least quasi harmonic behaviour of the potential. Obviously, this is not the case.
As can be seen from the data, the general trends are visible, but statistics is still rather poor. This is mainly due to the loss of 30 % of our beam time due to problems in the storage ring. All data here have been taken in only 6 shifts. After improving the statistics in a further experiment we want to determine the vibrational entropy, the capacity of heat and obtain the Grueneisen parameters. It would be very interesting to compare those results to data measured on alloys with different composition, in particular outside the range of the invar behaviour.

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