Fe_3Pt, an example for phonon softening at the structural phase transition

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Introduction

During the last few years, nuclear inelastic absorption (NIA) [1] has been established as a new and fruitful technique to probe phonons. This report presents phonon densities of states (DOS) of the invar alloy Fe_3Pt measured with NIA and compares these data with a DOS determined by coherent inelastic neutron scattering.

Methods and Materials

We have determined the vibrational density of states of Fe_3Pt at different stoichiometries, different states of order, and in a temperature range from 16 K to 300 K. With the temperature-dependent DOS, we were able to trace a phonon softening in the TA_1[110] branch of ordered FePt alloys around the stoichiometry Fe_3Pt [2, 3, 4]. Furthermore we found differences between the partial DOS, measured by means of nuclear inelastic absorption, and the total DOS measured by neutrons [2].

Discussion

Inspection of the phase diagram (Figure 1) shows the appearance of a tetragonal strained phase at low temperatures. This is due to a phonon instability in the TA_1[110] branch (i.e., a phonon softening) [5]. When o-$Fe_{75}Pt_{25}$ is cooled, the soft mode becomes visible (Figure 2). For the disordered lattice, this effect is small but visible (Figure 3).

In the ordered $Fe_{75}Pt_{25}$ phase, the cut-off frequency of the DOS changes only slightly with temperature. In the disordered phase, the cut-off frequency is reduced by approximately 2 meV if the temperature is increased from 150 K to 300 K. However, not only the cut-off frequency changes; the DOS at 300 K between 15 meV and 35 meV softens in general. This can be understood as a result from thermal lattice expansion.

A still puzzling feature appeared by approaching the martensitic phase transition from $L1_2$ (Cu_3Au) to bcc at room temperature (Figure 4). The DOSs of o-$Fe_{72}Pt_{28}$ and o-$Fe_{75}Pt_{25}$ do not differ a lot. Yet if the composition is changed by just one atomic percent, the weight of the low-frequency modes decreases. A structural analysis by x-ray diffraction shows only small changes. Neither the intensity (a measure for the degree of order and structure) nor the position of the diffraction peaks (indicating the lattice parameter) of o-$Fe_{76}Pt_{24}$ differs much from the diffraction pattern of o-$Fe_{72}Pt_{28}$ and o-$Fe_{75}Pt_{25}$. An analysis of the magnetic structure of o-$Fe_{76}Pt_{24}$ was less helpful because the material is quite close to the Curie temperature (indicated by T_C in Figure 1). The conversion electron Mössbauer

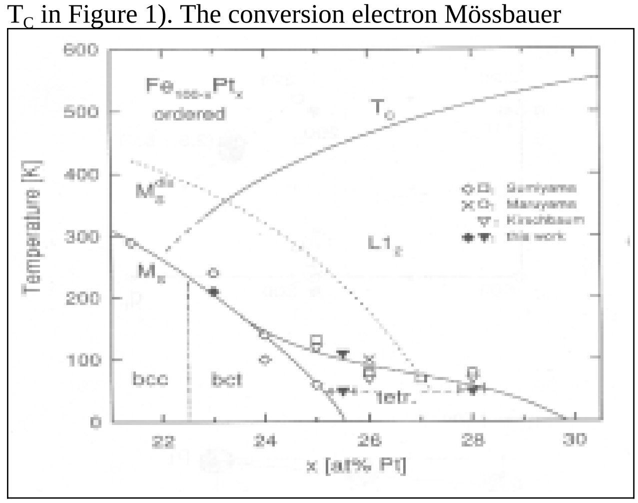

Figure 1: Magnetic and structural phase diagram of o-$Fe_{100-x}Pt_x$ taken from [5]; T_C is indicating the Curie temperature, M_S the martensitic phase transition from $L1_2$ (respectively tetragonal strained Cu_3Au) to bcc (respectively bct). The dashed line marks the martensitic phase transition for disordered $Fe_{100-x}Pt_x$.

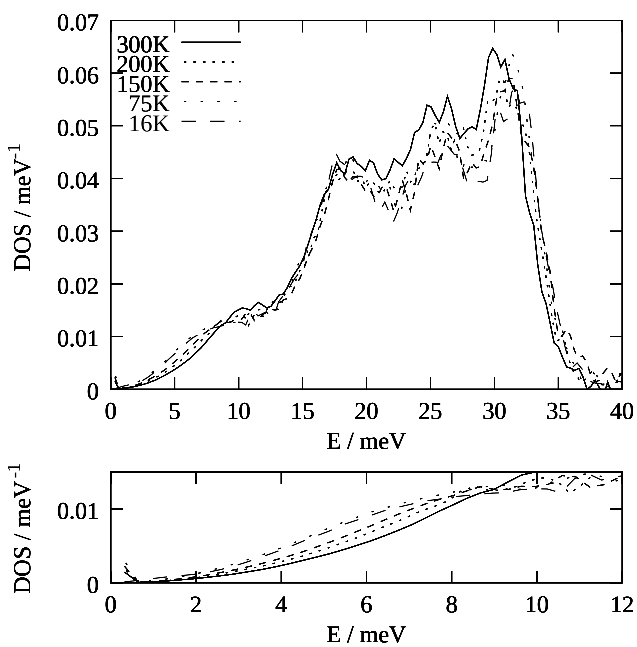

Figure 2: DOS of o-$Fe_{75}Pt_{25}$ at different temperatures.

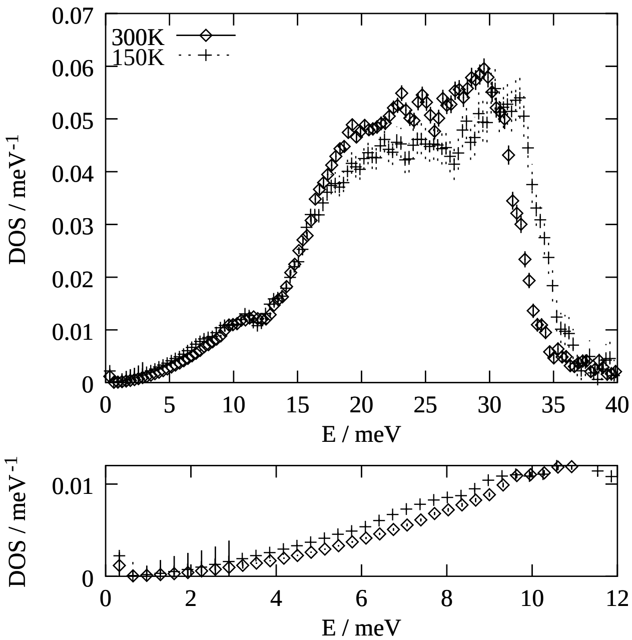

Figure 3: DOS of d-$Fe_{75}Pt_{25}$ at 150 K and 300 K.

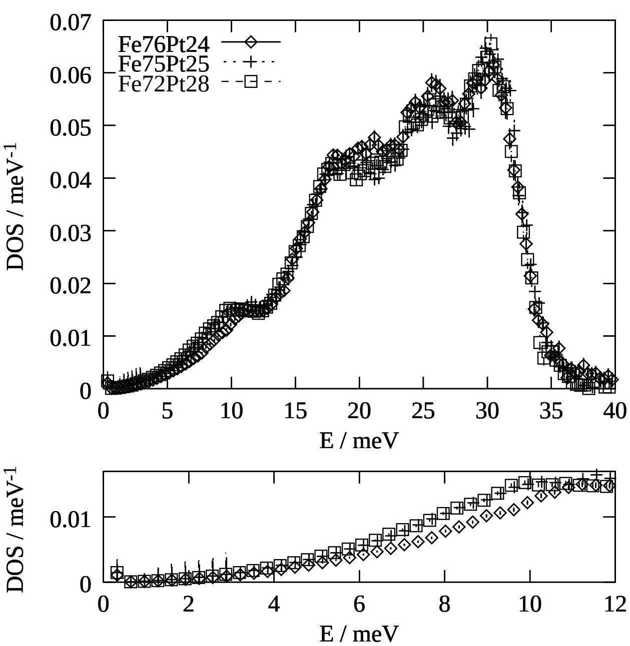

Figure 4: DOS of o-$Fe_{100-x}Pt_x$ at different temperatures; bigger errorbars below 3meV are due to the subtraction of the elastic line.

spectrum shows just a collapsing hyperfine field, a typical feature of ferromagnetic materials close to the Curie temperature. By comparing our data with the total DOS as measured by inelastic neutron scattering (Figure 5), we find that the modes with lowest frequencies are strongly suppressed in the ^{57}Fe DOS as compared to the neutron data. This is due to the resonant character of NIA, which just probes vibrations of the ^{57}Fe nuclei. In contrast, the neutron measurements [2] were sensitive to the Fe and Pt motions with almost the same weight because of the very similar coherent cross section of these elements.

The low-frequency modes contain mainly contributions from Pt due to its high mass, whereas the high-frequency modes correspond to optical vibrations where strong Pt-Pt and strong Fe-Fe forces play an important role.

Results

Here we demonstrate the potential of inelastic nuclear absorption in combination with inelastic neutron scattering to separate the element specific contributions to the total phonon density of states.

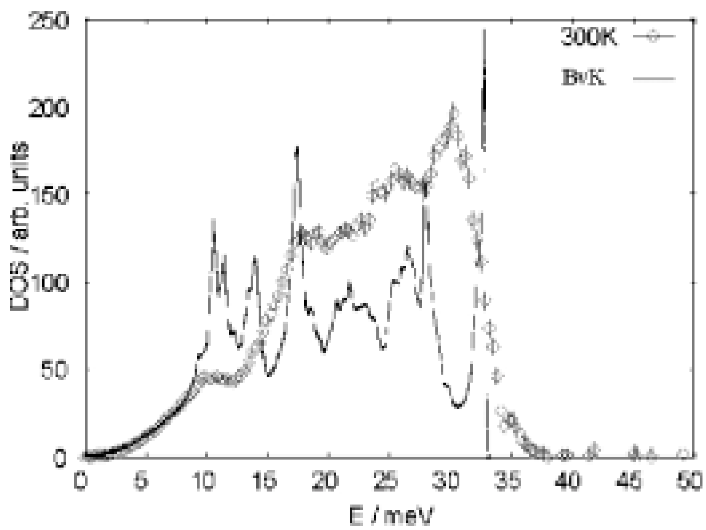

Figure 5: DOS of o-$Fe_{72}Pt_{28}$ measured by NIA at the APS and with neutrons [2] (in order to be able to compare the DOS conveniently the y-scale of the two datasets are different and therefore in arbitrary units).

Acknowledgements

We wish to thank E.E. Alp and W. Sturhahn at the Advanced Photon Source for the opportunity to use the 3-ID beam line. Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Basic Energy Sciences, Office of Science, under Contract No. W-31-109-Eng-38.

References

[1] M. Seto *et al.*, *Phys. Rev. Lett.* **74** (19), 3828–3831 (1995).
[2] Y. Nado *et al.*, *J. Phys. Soc. Japan* **57** (12), 4225–4231 (1988).
[3] J. Kästner *et al.*, *Eur. Phys. J. B* **10**, 641–648 (1999).
[4] N. Wiele *et al.*, *Physika B* **263–264**, 716–718 (1999).
[5] J. Kästner *et al.*, *Eur. Phys. J. B* **11**, 75–81 (1999).