Raman study of FeSi under high pressures up to 34 GPa

Ivan Jursic[1], Dirk Menzel[1], Joachim Schoenes[1] and Klaus Doll[2]

[1]Institut für Physik der Kondensierten Materie, Technische Universität Braunschweig, Germany
[2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

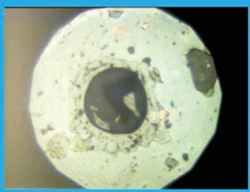
Introduction

FeSi is a narrow-gap semiconductor with unusual electronic properties. This led to the assumption that this material may belong to the class of Kondo insulators.

We performed micro-Raman measurements at pressures up to 34 GPa in a diamond anvil cell. Those measurements are then compared to DFT calculations.
An analysis of the frequency shifts as well as of the change of the spectral weight is performed.

Experimental details

Single crystals of FeSi were grown by the tri-arc Czochralski technique. These crystals were investigated by Raman spectroscopy in a diamond anvil cell at pressures up to 34 GPa.



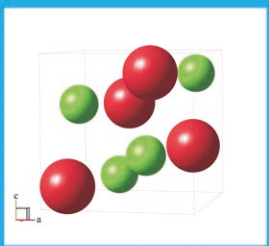
The experiment was performed at room temperature, and Daphne 7373 was used as a pressure transmitting medium. The sample size is approx. 80x60x40 µm, and the laser spot is 10 µm in diameter.

Structure of FeSi and factor group analysis

FeSi crystallizes in the B20 structure, i.e. space group P2,3. Factor group analysis yields the following Raman active modes

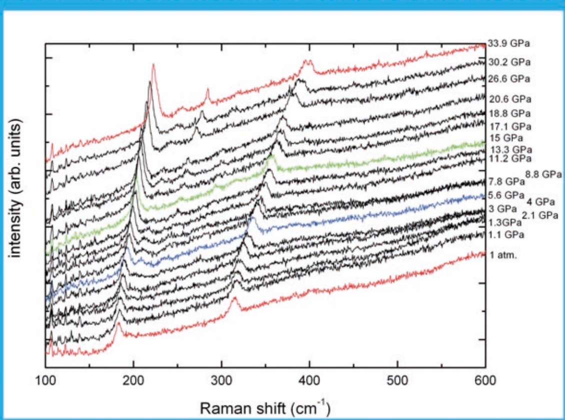
$$\Gamma = 2A + 2E + 5T$$

Previous measurements outside of the diamond anvil cell allowed the assignment of all the vibrations and showed an electron-phonon coupling for the E-mode at 180 cm^{-1}.[1]



The B20 structure

Raman measurements up to a pressure of 34 GPa

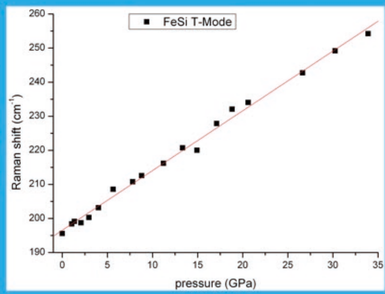


An overview of the Raman spectra at different pressures from 1 atm. up to 34 GPa.

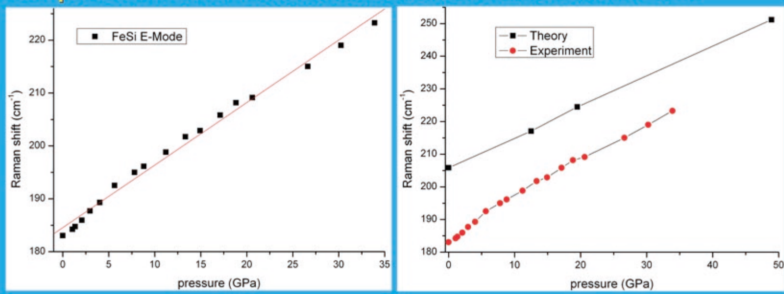
Change of T-mode vibration frequencies at different pressures

The frequency of the T-mode vibration, which is 195 cm^{-1} at ambient pressure, linearly increases with pressure.

There is no indication of a phase transition up to a pressure of 34 GPa.



Comparison with DFT calculations for the E-mode at 180 cm^{-1}

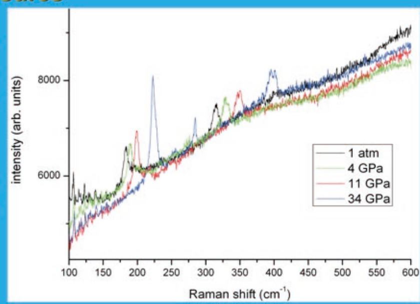


E-mode vibration frequencies at different pressures. Small kinks can be observed at 5 GPa and 15 GPa. The right panel displays a comparison between experimental (red) and theoretical (black) values. The theoretical frequencies were calculated within a DFT model.

Spectral weight at different pressures

When looking at the low frequency region the intensity of the background drops as pressure is increased.

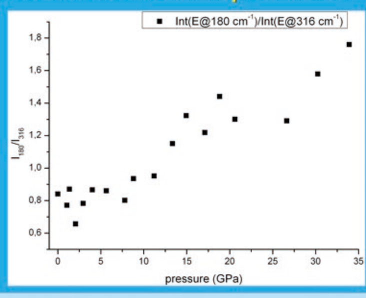
This is an indication of some correlation effects, but they are not as large as in Kondo insulators. [2][3]



Intensity of the E-mode vibrations at 180 cm^{-1} at different pressures

The intensity of the E-mode vibration which is 180 cm^{-1} at 1 atm is normalized to the E-mode vibration at 316 cm^{-1}.

The ratio I_{180}/I_{316} is 0.8 for low pressures and starts to increase at 5 GPa. It is getting larger than unity at pressures greater than 10 GPa.



Conclusions

We present micro-Raman studies on FeSi at pressures up to 34 GPa. Below this pressure no phase transition is observed. The phonon frequencies show small kinks at around 5 GPa and 15 GPa, but in general the frequency shifts agree with calculations made in a single particle model.

The change of the spectral weight can be interpreted as an indication for some correlation effects. The changes are too small to fit into a strongly correlated, i.e. Kondo insulator model and have to be further analyzed.

References

[1] A.-M. Racu et. al., Phys. Rev. B **76**, 115103 (2007)
[2] J.K. Freericks et. al., Phys. Rev. B **64**, 125110 (2001)
[3] P. Nyhus et. al., Phys. Rev. B **55**,12488 (1996)