Abstract

Rainer Lübbers:
"Magnetism and Lattice Dynamics under High Pressure Studied by Nuclear Resonant Scattering of Synchrotron Radiation."

This thesis is concerned with two new methods of nuclear resonant scattering of synchrotron radiation for the investigation of magnetism and lattice dynamics under high pressure. For this purpose a new generation of diamond-anvil cells has been developed which applies for the specific needs for (i) nuclear forward scattering (NFS), the analogue of the Mössbauer effect, and for (ii) nuclear inelastic scattering (NIS), a new method to determine the density of phonon states in solids.

(i) The NFS experiments were performed on magnetic Laves phases with the composition RFe_2 (R = Y, Gd, Sc) up to pressures of 1 Mbar (= 100 GPa). This pressure range allowed the study of iron magnetism in these model systems with a large variation of interatomic Fe-Fe distances. The competing variation of exchange interactions and Fe band moments is reflected by a systematic change of the magnetic ordering type from ferromagnetism with well-localized Fe moments via antiferromagnetism with more itinerant Fe moments to a non-magnetic state. This behaviour is similar to the observations in elemental iron (γ-Fe), when the lattice parameter is changed. We conclude from comparative studies on $ScFe_2$ that the antiferromagnetic state can only be obtained after a pressure-induced structural phase transformation from the cubic C15 to the hexagonal C14 structure.

It is further demonstrated that the variety of different magnetic phenomena in the RFe_2 series with non-magnetic R atoms can be reproduced by a single model system, namely YFe_2, when exposed to high pressure. A comparison with $GdFe_2$, exhibiting large Gd 4f moments, indicated a strongly increased interaction between the Fe and the Gd sublattices under pressure, which leads to a stabilization of the Fe moment.

(ii) The objective of the second part of the thesis is the first application of NIS for the study of phonons in iron under pressure. With a new high-pressure technique, based on a Be gasket for sufficient transmission of low-energy Fe $K_{\alpha,\beta}$ x-rays, the phonon density of states in the ε-phase of iron was experimentally determined for the first time. Since ε-Fe is the main component of the Earth's inner core, the results have direct geophysical impact. The NIS study provides values for the sound velocities and the pure vibrational contribution to a variety of thermodynamic properties like the Helmholtz free energy, the specific heat and the entropy. The present results can be used to test theoretical *ab initio* calculations, which model the physics of the Earth's core.