Phonon DOS in oriented hcp iron and SnO from high-pressure NIS

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This talk will first give an introduction to the methodological aspects connected with nuclear inelastic scattering (NIS) of synchrotron radiation (SR) for phonon spectroscopy using the Mössbauer resonances of Fe-57 and Sn-119, present the experimental set-up and a specially designed high-pressure cell.

The properties of the hexagonal high-pressure phase of iron, ε-Fe, are of actual geophysical interest. In continuation of previous Fe-57 NIS studies [1,2], very recent results on the phonon DOS of ε-Fe studied up to 130 GPa are presented. It is well known that ε-Fe, when pressurized in a diamond anvil cell, exhibit texture with a preferred alignment of the hexagonal c-axis parallel to diamond anvil axis [3]. NIS spectra measured parallel and almost perpendicular to the axis of the diamond anvils exhibit different spectral features; from difference spectra it is then possible to extract the phonon density-of-states (DOS) of ε-Fe as seen parallel and perpendicular to the hexagonal c-axis, as demonstrated in a recent NIS study of ε-Fe up to 40 GPa [4]. This allows for a mode-specific analysis of the phonon spectra, for instance an identification of the two optical modes and provided the first experimental proof of an anisotropy in the average sound velocity, v_D, parallel and perpendicular the hexagonal c-axis. Using the known bulk and shear moduli of ε-Fe, the compressional wave velocity v_p and the shear-wave velocity v_s can be obtained from the observed v_D values. A characteristic difference is again obtained, v_p is somewhat faster along the c-axis than perpendicular to it, in agreement with ab-initio calculations for the low temperature case [5]. The present results will be compared with results from other methods [6-8].

SnO has a graphite-like structure, and it is very easy to prepare from SnO grains a strongly oriented absorber with the tetragonal c-axis perpendicular to the absorber plane. NIS spectra taken at ambient conditions and different directions with respect to the c-axis were used to derive in the same way as described above the local phonon DOS as seen parallel and perpendicular to the c-axis. Applying pressure up to 6 GPa leads to a weakening of the pronounced difference of the projected DOS in the two different directions. In addition, a hardening of a soft phonon mode with pressure is observed. This behavior effect is explained by the graphite-like structure of SnO with weak Van-der-Waals forces between the plains and strong covalent binding within the plains. With increasing pressure the difference in binding strength and the strongly anisotropic elastic properties decreases, in accordance with a high-pressure XRD and EXAFS study [9].

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