

ANGULAR RESOLVED DENSITY OF PHONON STATES

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Inelastic nuclear absorption of synchrotron radiation has proven to be a new method for studying lattice dynamics. So far polycrystalline, amorphous and fluid samples were investigated where one gets the information on lattice dynamics in an integral form, i.e. the modes of vibrations along various directions are averaged. Here we measure separately the frequency distribution of lattice vibrations along different crystallographic directions.

We have measured the energy spectra of inelastic absorption of 14.4 keV synchrotron radiation in a ferric borate $^{57}\text{FeBO}_3$ single crystal for several polar angles θ and azimuthal angles φ between the incident x-ray beam and the [111] axis (Figure 1). The

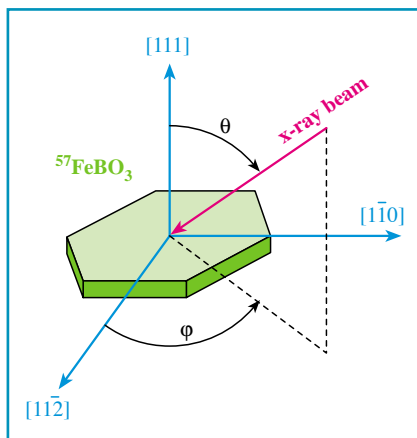
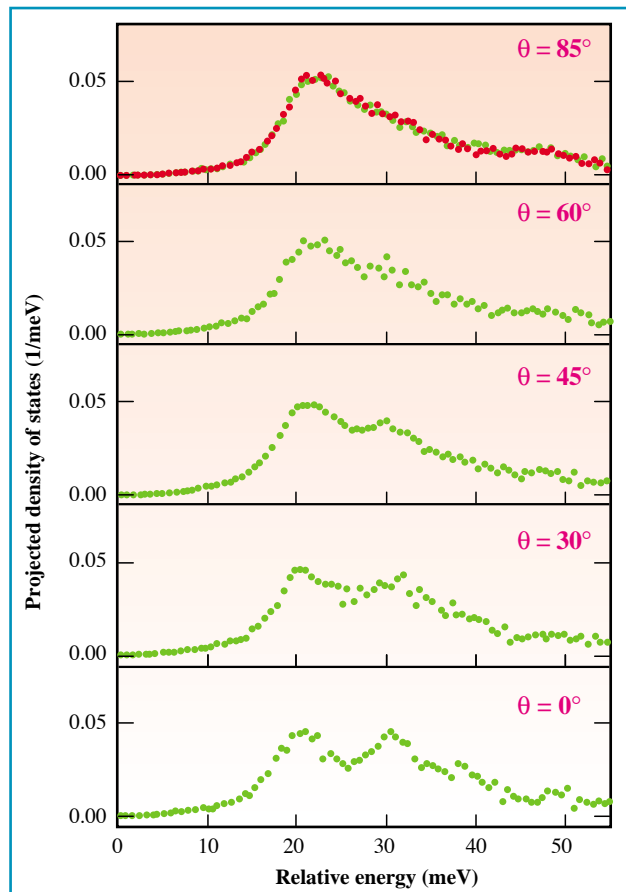


Fig. 1: Orientation of the incident x-ray beam relative to the crystal.

frequency distributions of lattice vibrations along these directions (i.e., projected densities of phonon states) were derived and the Lamb-Mössbauer factors for each case were calculated.

Derived projected densities of states are shown in Figure 2. They give the frequency distribution of lattice vibrations, weighted by the projection of the phonon polarization vector to the direction of the x-ray beam. The densities of phonon states show a pronounced dependence on the polar angle. When the polar angle is high ($\theta = 85^\circ, 60^\circ$) the densities of states

Fig. 2: The projected densities of phonon states along several crystallographic directions. The polar angles θ for various directions are indicated in the Figure. The data for the azimuthal angle $\varphi = 90^\circ$ are shown with green circles and for $\varphi = 0^\circ$ with red circles.



have one peak at about 20 meV. When the angle decreases ($\theta = 45^\circ, 30^\circ$, and 0°) this peak remains, but an additional peak appears at about 30 meV. In contrast to the sensitivity of the densities of states to the polar angle, the spectra at two azimuthal angles ($\varphi = 90^\circ$ and 0°) coincide.

For all crystal orientations, the calculated Lamb-Mössbauer factors are 0.82(2). In contrast to the pronounced anisotropy of the projected densities of states they do not depend on the crystal orientation. Although this is a surprise, it is not a contradiction, because the Lamb-Mössbauer factor is not very sensitive to the details of the density of phonon states. The constant value of the Lamb-Mössbauer factor along six non-equivalent crystallographic directions gives strong indication that the mean-square displacement of the iron atoms in the ferric borate crystal is mostly

isotropic with a value of $0.0042(5) \text{ \AA}^2$. In this concern we note that our results do not confirm the large anisotropy of the mean-square displacement reported earlier on the basis of crystal structure refinement.

The observed combination of the pronounced anisotropy of the density of phonon states and the isotropic mean-square displacement of the iron atoms give a striking example of the advantages of the nuclear inelastic absorption technique compared, for example, to Mössbauer spectroscopy, where the Lamb-Mössbauer factor is the only parameter to study the lattice dynamics. ■

REFERENCES

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