

Vibrational properties on CuFeS₂ under high pressure

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An insulator-metal transition is one of the interesting properties in strongly correlated electron systems. At ambient pressure, CuFeS₂ is an antiferromagnetic semiconductor. As indicated by high-pressure resistivity measurements at room temperature, it undergoes the insulator-metal transition at 6.5 GPa with increasing pressure. Furthermore, the antiferromagnetic order disappears at this transition.

In the present study, we have measured X-ray diffraction and ⁵⁷Fe nuclear resonant inelastic scattering (NRIS) of CuFeS₂ under pressure using synchrotron radiation at SPring-8. The X-ray diffraction data were collected at room temperature with angle-dispersive techniques and an image-plate detector on BL10XU. For ⁵⁷Fe NRIS, the pulsed synchrotron radiation was monochromatized by the high-resolution monochromator on BL09XU. The ⁵⁷Fe NRIS spectra were measured by tuning the highly monochromatized X-ray beam in an energy range of about 80 meV.

Since a halo-like pattern is observed in the X-ray diffraction data above 6.3 GPa, CuFeS₂ undergoes a pressure-induced crystal-amorphous transition. ⁵⁷Fe NRIS spectra under pressure consist of large center peaks originating from elastic scattering and sidebands resulting from inelastic scattering with the annihilation and creation of phonons. The inelastic components in the spectra extract lead to the partial phonon densities of states (DOS) assuming a harmonic lattice model. There are three peaks at 10, 22 and 43 meV in the extracted partial phonon DOS below 6.0 GPa. It is noteworthy that the peak at around 10 meV in the phonon DOS stays almost unchanged up to 6.0 GPa.