Structural and vibrational properties on $CuFeS_2$ under pressure

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An insulator-metal transition is one of the interesting properties in strongly correlated electron systems. At ambient pressure, $CuFeS_2$ is an antiferromagnetic semiconductor. As indicated by high-pressure resistivity measurements at room temperature [1], it undergoes the insulator-metal transition at 6.5 GPa with increasing pressure. Furthermore, the antiferromagnetic order disappears at this transition [2].

In the present study, we have measured X-ray diffraction and ^{57}Fe nuclear resonant inelastic scattering (NRIS) of $CuFeS_2$ 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 ^{57}Fe NRIS, the pulsed synchrotron radiation was monochromatized by the high-resolution monochromator on BL09XU. The ^{57}Fe NRIS spectra were measured by tuning the highly monochromatized X-ray beam in an energy range of about 60 meV.

Since a halo-like pattern is observed in the X-ray diffraction data above 7.1 GPa, $CuFeS_2$ undergoes a pressure-induced crystal-amorphous transition. ^{57}Fe 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 5.5 GPa. The lowest peak originates from the acoustic phonon branches and other two peaks come from optical branches. Above 7 GPa, the acoustic and optical phonon branches are overlapped.

[1] G.D. Pitt and M.K.R. Vyas Solid State Commun. **15**(1974) 899.
[2] H. Kobayashi, H. Onodera, and T. Kamimura Hyperfine Interact. (C) **5**(2002) 165.