High –pressure Phase Transition in Laboratory Synthesize Orthorhombic $CuFe_2S_3$: Mössbauer Studies Up to 7 GPa

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Natural orthorhombic cubanite transforms to more stable isocubanite having FCC-Fm3m structure (1) at ~200C and between 3.8 – 5.2 GPa. Due to unique physico-chemical condition needed, $CuFe_2S_3$ could not be synthesized in the laboratory in orthorhombic form. An attempt to synthesize the system in laboratory using resistive and microwave heating techniques is reported. XRD patterns show the presence of orthorhombic cubanite for microwave synthesized sample while pattern for resistive heated sample indicate isocubanite in abundance. High pressure Mössbauer measurements carried out on resistive heated sample using Diamond Anvil Cell (2) indicates the importance of preparatory methods to maintain the physico-chemical conditions (3). The magnetic hyperfine field of ~33T at ambient conditions corresponds to orthorhombic phase contradicting the XRD analysis. The magnetic sextet transforms into a doublet at ~ 4.2 GPa (Fig.1). The isomer shifts of 0.22 and 0.77 mm/sec (with reference to α-Fe) correspond to high spin Fe^{3+} and Fe^{2+} in tetrahedral coordination. The pressure induced electrical resistivity measurements also support the first order phase transition at ~ 4 GPa confirming the synthesis of orthorhombic cubanite (4).

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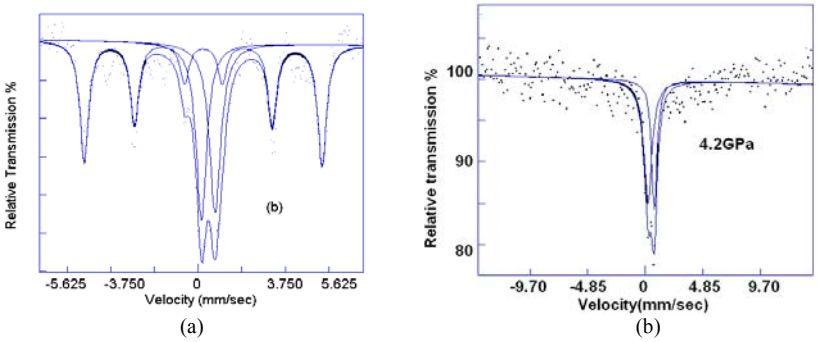

(a) (b)

Figure 1. Room Temperature Mössbauer spectra of synthesized cubanite using resistive heating technique at (a) ambient pressure (b) 4.2 GPa.