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ABSTRACTS







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F5-08. Crystalline Structure and Magnetic Properties of Pyrite FeS₂.

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Iron pyrite (FeS₂) are recognized significant attention as promising inorganic materials applications, such as electrode materials for high-energy batteries, medical diagnostics, semiconductor materials, and photovoltaic solar cells. In this paper, we provide that the crystalline structure and magnetic properties of pyrite FeS2 were characterized with X-ray diffraction (XRD), vibrating sample magnetometer (VSM), and Mössbauer spectroscopy. From the refined XRD patterns, it was confirmed that the crystalline structure of FeS₂ was cubic pyrite (Pa-3 space group) with the lattice constants of $a_0 = 5.4176$ Å. The hysteresis loops of FeS₂ were measured by VSM in the maximum applied field of 10 kOe at 4.2 and 295 K. As shown in Fig. 1, the saturation magnetization at 4.2 and 295 K was 0.123 and 0.035 emu/g, respectively. Mössbauer data were collected in the temperature range of 4.2-500 K. The spectra at all temperature were fitted one-doublet. The Mössbauer spectra of FeS2 at 4.2 and 295 K are shown in the inset of Fig. 1. The electric quadrupole splitting ($\Delta E_{\rm O}$) values are 0.63 and 0.60 mm/s for 4.2 and 295 K, respectively. The ΔE_0 values with decreasing temperatures increases slightly due to changes in the Fe-S distance. The isomer shift (δ) values are 0.28 and 0.18 mm/s for 4.2 and 295 K, indicating the Fe3+ state. The temperature dependence of δ values is due to the second order doppler shift.

[1] Z. Meng, F. Wei, W. Ma, etc., Adv. Funct. Mater., Vol. 26, p.8231 (2016).

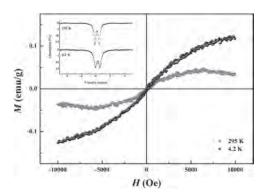


Fig. 1. Hysteresis loops and Mössbauer spectra of FeS₂ at 4.2 and 295 K.