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Investigations on FeSb₂ by high field ⁵⁷Fe Mössbauer spectroscopy

FeSb₂ has gained much interest in recent years, because of its potential as a thermoelectric material. It is a nearly ferromagnetic small gap semiconductor with a semiconductor-metal transition above 80 K [1]. It crystallizes in the marcasite structure, where Fe has only one crystallographic site, surrounded by distorted Sb-octahedra [2]. These octahedra are corner shared in the ab-plane and edge sharing along the c-axis. With decreasing temperature the distortion of the octahedra increases, showing a maximum around 100 K [3]. At low temperatures the material is diamagnetic. With increasing temperature a paramagnetic-like behavior is observed. The aim of this work is to get more information about the magnetic state of the iron atom in this compound. We report on ⁵⁷Fe Mössbauer investigations in zero and in applied fields up to 13.5 T at temperatures between 4.2 K and RT on polycrystalline FeSb₂ samples enriched with Fe-57. The spectra were analysed by solving the full Hamiltonian, taking into account both electrostatic and magnetic interactions, as well as the sample thickness. The zero field spectra can be fitted by only one subspectrum, with a quadrupole splitting which increases with decreasing temperature, reaching a maximum at about 50 K. In contrast to this the in-field spectra are extremely complex. Several models were tested to explain the spectra. At least 5 subspectra is necessary with line widths for some of them indicating that this is only a minimum number. Common to all models is that the mean values for quadrupole splitting and center shift fit well to the zero-field results. [1] A.V. Lukoyanov et al., Eur.Phys.J. B 53, 205 (2006).[2] F. Hullinger, Struct. Bonding (Berlin) 4, 83 (1967).[3] C. Petrovic et al., Phys.Rev.B 72, 045103 (2005).

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