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Crystallographic and Mössbauer Studies for $Ni_{0.99}{}^{57}Fe_{0.01}Ga_2S_4$

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$Ni_{0.99}{}^{57}Fe_{0.01}Ga_2S_4$ was fabricated by using a solid-state method with high-purity elements of Fe, Ni, Ga and S. The structure of the sample was examined with an X-ray diffractometer (XRD) and analyzed by using the Rietveld refinement. The crystal structure of the $Ni_{0.99}{}^{57}Fe_{0.01}Ga_2S_4$ was determined to be a trigonal structure of P-3m1 with lattice constants $a_0 = 3.629$ Å, $b_0 = 3.629$ Å and $c_0 = 11.996$ Å. The Mössbauer spectra of $Ni_{0.99}{}^{57}Fe_{0.01}Ga_2S_4$ were recorded at various temperatures ranging from 4.2 to 300 K. The magnetic hyperfine field and the electric quadrupole interactions at 4.2 K were fitted, yielding the following results: $H_{hf} = 112.7$ kOe, $\Delta E_Q = 1.374$ mm/s, $\theta = 48.0°$, $\varphi = 0.0°$, $\eta = 0.5$ and $R = 1.8$. The charge state of Fe ions is ferrous (Fe^{2+}) as characterized by an isomer shift of $\delta = 0.653$ mm/s at 300 K. The Mössbauer spectra show a large quadrupole interaction in $Ni_{0.99}{}^{57}Fe_{0.01}Ga_2S_4$.

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