Electric quadrupole interaction in cubic BCC $\alpha$-Fe

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Mössbauer transmission spectra for the 14.41-keV resonant line in $^{57}$Fe have been collected at room temperature by using $^{57}$Co(Rh) commercial source and $\alpha$-Fe strain-free single crystal as an absorber. The absorber was magnetized to saturation in the absorber plane perpendicular to the $\gamma$-ray beam axis applying small external magnetic field. Spectra were collected for various orientations of the magnetizing field, the latter lying close to the [110] crystal plane. A positive electric quadrupole coupling constant was found practically independent on the field orientation. One obtains the following value $V_{zz} = +1.61(4) \times 10^{19}$ Vm$^{-2}$ for the (average) principal component of the electric field gradient (EFG) tensor under assumption that the EFG tensor is axially symmetric and the principal axis is aligned with the magnetic hyperfine field acting on the $^{57}$Fe nucleus. The nuclear spectroscopic electric quadrupole moment for the first excited state of the $^{57}$Fe nucleus was adopted as +0.17 b. Similar measurement was performed at room temperature using as-rolled polycrystalline $\alpha$-Fe foil of high purity in the zero external field. Corresponding value for the principal component of the EFG was found as $V_{zz} = +1.92(4) \times 10^{19}$ Vm$^{-2}$. Hence, it seems that the origin of the EFG is primarily due to the local (atomic) electronic wave function distortion caused by the spin-orbit interaction between effective electronic spin $S$ and incompletely quenched electronic angular momentum $L$. It seems as well that the lowest order term proportional to the product $L \cdot \lambda \cdot S$ dominates, as no direction dependence of the EFG principal component is seen. The lowest order term is isotropic for a cubic symmetry as one has $\lambda = \lambda \cdot 1$ for cubic systems with the symbol 1 denoting unit operator and $\lambda$ being the coupling parameter.

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