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Temperature dependences of the hyperfine parameters of Fe^{2+} in $FeTiO_3$ as determined by ^{57}Fe-Mössbauer spectroscopy

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Abstract

The temperature variations of the ferrous Mössbauer parameters for a synthetic ilmenite ($FeTiO_3$) have been determined and interpreted over a very wide temperature range (5–900 K). The Debye model of the lattice vibrations was used in interpreting the temperature dependence of the center shift, yielding a characteristic Mössbauer temperature of 350 ± 20 K and a zero-Kelvin intrinsic isomer shift of 1.30 ± 0.01 mm/s. The temperature dependence of the ferrous Mössbauer quadrupole splitting was interpreted using crystal field theory. A most adequate description of the experimental $\Delta E_Q(T)$ curve was obtained assuming an energy shift of at the most ca. 500 ± 50 cm^{-1} for the highest orbital T_{2g} level relative to the lowest level within this T_{2g} triplet. The temperature dependence of the hyperfine field was interpreted within the molecular field theory of magnetism assuming the magnetic exchange energy being a function of interatomic spacing, indicating a first-order magnetic transition at the magnetic-paramagnetic transition temperature of 59.0 ± 0.5 K.

This detailed presentation of Mössbauer parameters as a function of temperature can serve as a basis for easily detecting ilmenite ore at, for example, the lunar surface and for monitoring by means of Mössbauer spectroscopy the reduction process of the mined mineral, for the purpose of supplying a future Moon base site with oxygen and water.

Keywords: Ilmenite, Mössbauer spectroscopy, hyperfine interactions, temperature variation, Moon base