Electric Quadrupole Interactions of the Short-Lived β -Emitter ¹²N in Insulator Crystals (¹²N Implanted in Single Crystal TiO₂)*

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The electronic structure of nitrogen atoms as impurities in an ionic TiO_2 crystal has been investigated by analyzing electric field gradients (EFGs) measured by use of short-lived β -emitting ^{12}N implanted following nuclear reactions. Conventional β -NMR and its modification, suitable for the detection of quadrupole effects in the NMR spectra, were used for the investigation of hyperfine interactions of ^{12}N located in substitutional sites of O atoms and interstitial sites in the crystal. In order to deduce absolute values of the EFGs from the obtained eqQ/h, the quadrupole moment of ^{12}N has been determined from the NMR detection of ^{12}N implanted in BN(hexagonal) crystal. Here the EFG at the N atom in BN was measured by detecting the FT-NMR of ^{14}N in the crystal. The EFGs in TiO_2 are compared with the theoretical predictions based on the ab initio band-structure calculation in the framework of the KKR method.

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