Electric Quadrupole Interactions of the Short-Lived $\beta$-Emitter $^{12}$N in Insulator Crystals ($^{12}$N Implanted in Single Crystal TiO$_2$)*

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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 $\beta$-emitting $^{12}$N implanted following nuclear reactions. Conventional $\beta$-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 $eqQ/l$, 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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