

Lattice sites of ^{23}Ne implanted in single-crystal ZnO studied by β -NMR/NQR spectroscopy

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Zinc oxide is a II-VI binary compound that crystallizes in a hexagonal wurtzite structure. The compound has received significant attention because of its potential for application in optoelectronic devices and transparent conducting films as well as in space environments owing to its radiation hardness. In particular, owing to wide and direct band gap of 3.4 eV at room temperature, ZnO can be utilized in next-generation devices for short-wavelength optoelectronics such as light-emitting diodes operating in the spectral range from blue to ultraviolet. For utilizing ZnO as semiconductors, both *n*-type and *p*-type doped ZnO are necessary. We can fabricate *n*-type ZnO through the partial substitution of Zn with Al, Ga, or In, whereas fabricating a reliable high-quality *p*-type ZnO still remains a challenge. Despite considerable research conducted so far, high-quality *p*-type ZnO has not been fabricated.

Recently, first-principles calculations performed by Malý *et al.* indicated that a noble gas (He, Ne, or Ar) implanted in ZnO can serve as a new type of dopant.¹⁾ In spite of its fully occupied atomic orbitals, the noble gas strongly changes the surrounding electronic states by pushing away the electrons around it. This suggests that a noble gas can be a functional dopant in ZnO, and the investigation of ZnO using noble-gas nuclei as local probes is much anticipated. In this study, we investigate, in particular, Ne implantation into single-crystal ZnO.

For details of the experimental setup, see our earlier report.²⁾ First, using the β -NMR method, we determined the nuclear *g*-factor for the radioactive ^{23}Ne isotope (nuclear spin $I = 5/2$) that decays through β -emission into the nucleus ^{23}Na with a half-life of $T_{1/2} = 37$ s. Thereafter, we implanted the ^{23}Ne isotopes as probe nuclei in ZnO and measured the electric field gradient (EFG) at the ^{23}Ne stopping sites using β -NQR method. EFGs are highly sensitive to the electronic density in the vicinity of the relevant nucleus. This sensitivity can be used to identify the crystallographic sites for the implanted ^{23}Ne and to study the effect of ^{23}Ne implantation on the charge distribution around the nucleus. The β -NQR spectrum obtained at 47 K is depicted in Fig. 1.

We determined the electric field gradient V_{zz} at the

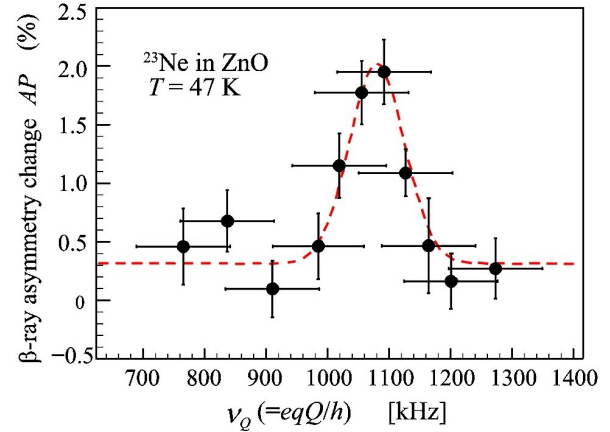


Fig. 1. β -NQR spectrum of ^{23}Ne implanted in ZnO single crystal. The dashed line represents the least χ -square fitting result to a Gaussian function.

position of ^{23}Ne in ZnO. The value of $(3.1 \pm 0.3) \times 10^{20}$ [V/m²] for ^{23}Ne compare well with that for ^{20}Na on the interstitial site (see Table 1). Although Ne occupies an octahedral interstitial site (the lowest energy site for Ne),¹⁾ Na in the form of ion (Na^+) is shifted by 0.23 Å from the ideal octahedral site parallel to the *c*-axis.⁶⁾ Considering that both Ne and Na^+ have the same electron configuration $1s^2 2s^2 2p^6$, we must study the position dependence of V_{zz} further in detail theoretically.

Table 1. Experimental results of the electric field gradient V_{zz} in ZnO for the β -NQR probes of ^8Li , ^{12}N , and ^{20}Na .

Implanted probe	^8Li ³⁾	^{12}N ⁴⁾	^{20}Na ⁵⁾
V_{zz} [10^{20} V/m ²]	1.342±0.001 interstitial site close to octahedral site	0.86 ±0.11 site unclear	2.7 interstitial site close to octahedral site ⁶⁾
Lattice site	0.6029±0.0004 Zn substitutional site		1.8 Zn substitutional site ⁶⁾

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