3_Ion implantation into beta-Gallium Oxide

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The ion implantation into beta-type gallium oxide, which is expected as a next-generation power semiconductor device will be explained [(1)].

Crystal structures

The MARLOWE code can handle single crystal structures. However, the structure of the target must be set accurately. The MARLOWE user must give the arrangement of atoms in the unit cell of the crystal, the binding energy, the Debye temperature that represents the vibration state of the crystal, and so on. The correct data cannot be given for the arrangement of atoms in the unit cell without understanding the symmetry of the crystal. Here, the information required to specify the crystal structure will be introduced. The MARLOWE can handle the following crystal systems.

1. Primitive
2. Body-centered
3. End-centered A
4. End-centered B
5. End-centered C
6. Face-centered

The gallium nitride mentioned last time is expressed as hP4. This is a simple lattice (Primitive) with a hexagonal structure, which means that it contains four atoms. The values of the crystal axis coordinates are as follows.

	x	y	Z
Ga	0.0	0.0	0.0
Ga	0.3333	-0.3334	0.5
N	0.0	0.0	0.3772
N	0.3333	-0.3334	-0.1228

The crystal structure of beta-type gallium oxide is mC20 in Pearson symbol. In this notation, the m stands for mono-clinic and the C stands for C centering. And 20 indicates that there are 20 atoms in the unit cell. Th C centering means the operation of translating the basic crystal to the center position of the C plane to create the original crystal structure. Specifically, the translation vector is (0.5, 0.5, 0). The specific crystal coordinates are summarized in the table below. The symmetry operation on this structure ultimately creates 20 lattice sites.

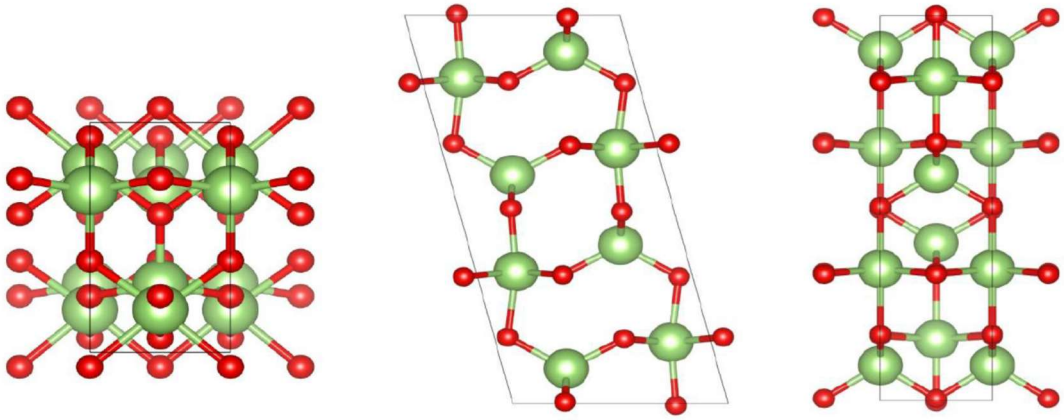
	x	y	z
Ga1	0.0904	0.0	0.2948
O1	0.1674	0.0	0.6011
O2	0.1721	0.0	0.0635
Ga2	0.3414	0.0	0.1857
O3	0.5043	0.0	0.2447
Ga1	0.9096	0.0	0.7052
O1	0.8326	0.0	0.3989
O2	0.8279	0.0	0.9365
Ga2	0.6586	0.0	0.8143
O3	0.4957	0.0	0.7553

For beta-type gallium oxide, the lattice constants are a-axis 12.2247 Å, b-axis = 3.0403 Å and c-axis 5.8088 Å. The angles formed by the crystal axes are α =90 degrees, β =103.82 degrees, and γ = 90 degrees. The volume of the gallium oxide unit cell is expressed by the following formula.

$$V = \frac{1}{2} abc\ sin\beta$$

From this equation, the volume is 209.356 Å^3. From this value, the atomic density is calculated as 9.55E22 n /cm^3.

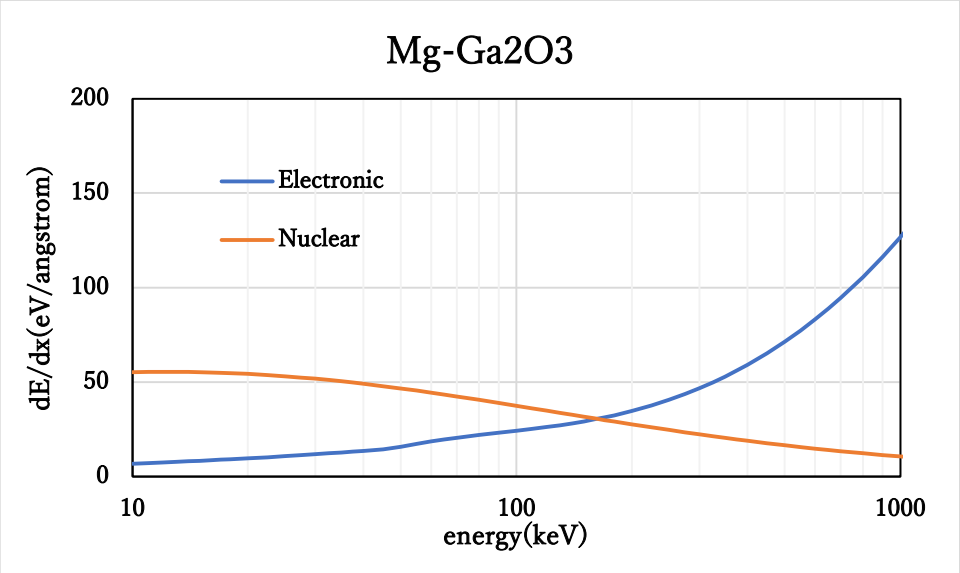
The crystal structure when viewed from each crystal plane is shown below. This crystal model was created by soft wafers called VESTA [(2)] and ReciPro [(3)].



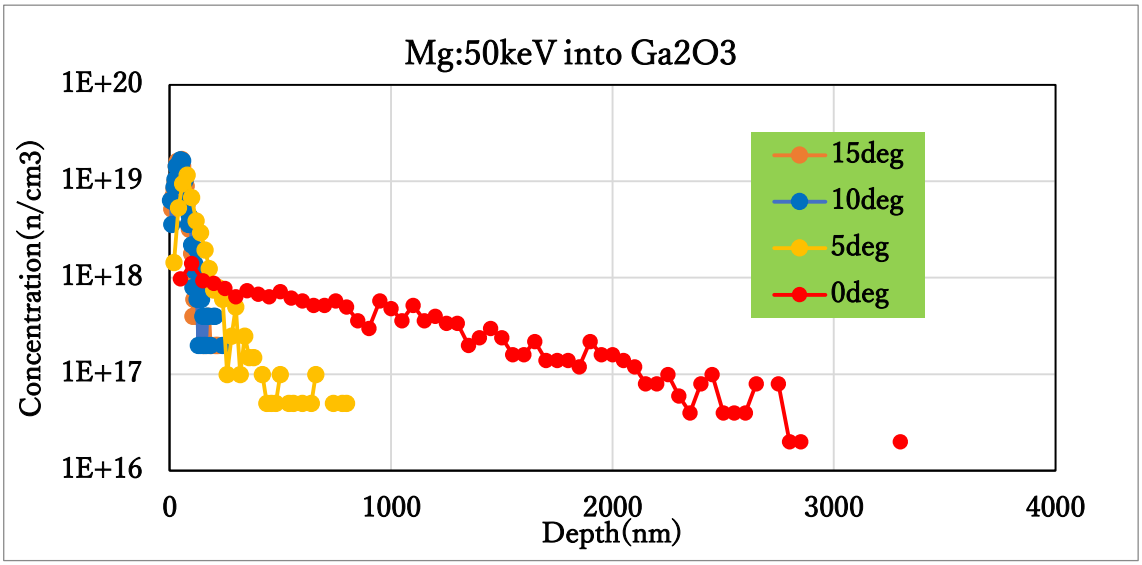
A-axis　　B-axis　　C-axis

Ion implantation into beta-Ga_2O_3

As explained in the previous article, the ion implantation phenomenon can be explained by the stopping power of the nucleus and the electronic stopping power. The following graph shows the stopping power of Mg implanted into gallium oxide using simulation code SRIM [4]. The energy at which the nuclear stopping power and the electronic stopping power match is around 180 keV. Below this energy, the stopping power of the nucleus is dominant, and above this energy, the electronic stopping power is dominant.

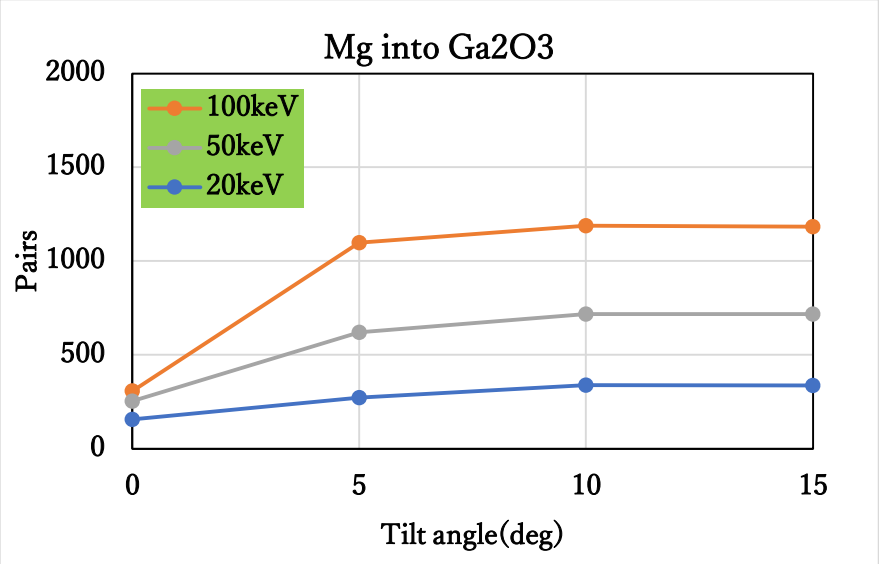


When ions are injected along the b-axis, a channeling phenomenon in which the ions pass deep into the substrate is likely to occur. The graph below shows the profile of ion implantation into beta-type gallium oxide. As can be seen from the profiles, the ion implantation along the b-axis causes channeling and penetrates to a depth of about 2 μm. However, the random implantation condition can be realized by setting the tilt angle, and channeling can be suppressed.



Ion implantation damage

Ion implantation damage can be explained by the number of Frenkel pairs produced by the collision. The following figure shows the results of investigating how the number of Frenkel pairs changes when the tilt angle is changed. When the energy is low, the number of Frenkel pairs does not increase significantly even if the tilt angle is changed. However, as the energy increases, the number of Frenkel pairs increases depending on the tilt angle, and the number of Frenkel pairs stabilizes at a tilt angle of 5 degrees or more.



As described above, the ion implantation phenomenon into gallium nitride was explained using the analysis results by the MARLOWE code. Ion implantation phenomena can be analyzed for other targets by specifying the crystal structure accurately.

References

1) Z. Hou, et. al., Electron devices Lett., 39, 6, 869(2018)
2) K. Momma and F. Izumi, "VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data," J. Appl. Crystallogr., **44**, 1272–1276 (2011)
3) http://pmsl.planet.sci.kobe-u.ac.jp/~seto/?page_id=19&lang=ja
4) http://www.srim.org/

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