Calculation of positron states and annihilation parameters in gamma and amorphous Al_2O_3

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Gallium nitride and related compounds attract much attention because of their applicability not only in light-emitting devices but also in power devices. The quality of gate insulator material plays a crucial role for the device performance and Al_2O_3 is a promising candidate. Recently, we applied slow positron beams in characterizing gate-stack Al_2O_3 layers [1]. It is thought that deposited Al_2O_3 layers have various structures depending on the preparation method and condition. In the present study, we construct appropriate structural models of gamma and amorphous Al_2O_3, which are often observed in real cases, and calculate positron states and annihilation parameters therein.

Gamma Al_2O_3 has a defect cubic spinel structure. To obtain a stoichiometric Al_2O_3, three cubic cells are needed. By removing 8 Al atoms, a stoichiometric $Al_{64}O_{96}$ structure is constructed. There are two different crystallographic Al sites in the cubic spinel structure, the octahedral (*O*) and tetrahedral (*T*) sites. Randomly removing 8 Al atoms from the *O* sites only or from both the *O* and *T* sites, we construct 16 different structural models and calculate positron states and annihilation parameters Figure 1 represents the calculated positron annihilation parameters and examples of the positron density distribution. Depending on the local structure, the obtained annihilation parameters differ slightly. The calculated positron lifetime values fall in the same range as the experimental results [1].

Amorphous Al_2O_3 structures are modeled by first-principles molecular dynamics using cubic cells containing 160 atoms therein with various lattice parameters. Positron annihilation parameters are obtained as a function of the density and systematic correlations are observed.

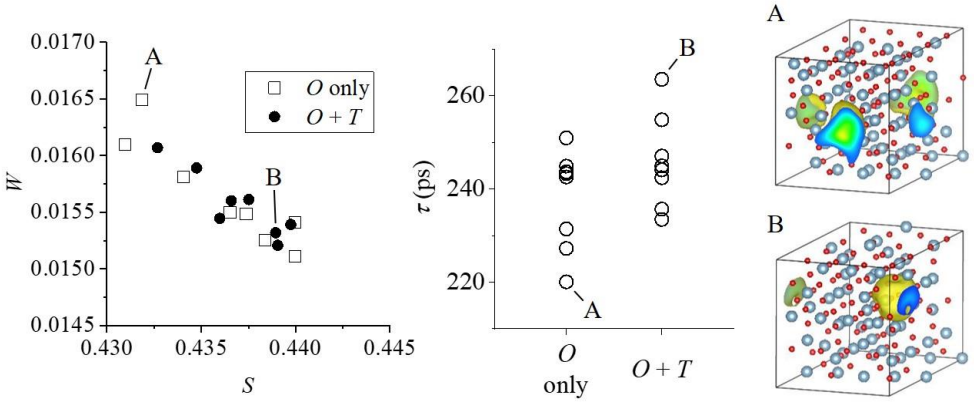

Figure 1 *Calculated positron annihilation parameters and examples of positron density distribution (corresponding to the parameters marked "A" and "B") in gamma Al_2O_3.*

References

[1] A. Uedono, T. Nabatame, W. Egger, T. Koschine, C. Hugenschmidt, M. Dickmann, M. Sumiya, and S. Ishibashi, J. Appl. Phys. **123**, 155302 (2018).

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