Two-component density functional calculations on lifetimes of positrons in a variety of crystals

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Positron annihilation technique (PAT) is well established as a tool to study vacancy type defects in a variety of solids. Especially, since slow positron beam technique enables detecting atomic defects of thin films, the PAT is widely used to evaluate the quality of device materials. Observation of positron lifetimes gives information on the size of atomic defects. To clearly identify the defects, reliable calculations on the lifetime is essential.

In this study, we implement the two-component density functional theory on the first-principles calculation code, PHASE, which is opened (http://www.rss21.iis.u-tokyo.ac.jp/index.html). In this program, both Troullier-Martin type soft pseudopotential and ultrasoft pseudopotential can be used and the plane wave basis set is employed. To confirm the validity of our method, we perform calculations on crystals by using the generalized gradient approximation for the electron many body effect and the local density approximation (LDA) for the positron-electron correlation [1]. For gap systems, we introduce the correction of the LDA by using the high-frequency dielectroric constant, where the imperfect screening of electrons is considered [2]. We carefully construct the pseudopotentials to reproduce electron charge in the interstitial region where the positron is located. As shown in Fig. 1, calculations well reproduce experimental results. We therefore conclude that the two-component density functional theory and the above mentioned correction for gap systems are useful to analyze the experimental results.

Hf oxide attracts technological interests as a high-k gate insulating film of the MOSFET device. The positron lifetime for the monoclinic crystal based on the LDA is found to be 146 ps which is much lower than the experimental value(170ps). By using the dielectric constant of 4, we correct the LDA and obtain the value of 157 ps. Thus, the correction improves the calculated value even in the case that the high-frequency dielectric constant is rather low and thus the screening effect is expected to be smaller than that of the homogeneous electron system.

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[1] M. J. Puska et al., Phys. Rev. B52, 10947 (1995).
[2] M. J. Puska et al., Phys. Rev. B39, 7666(1989).

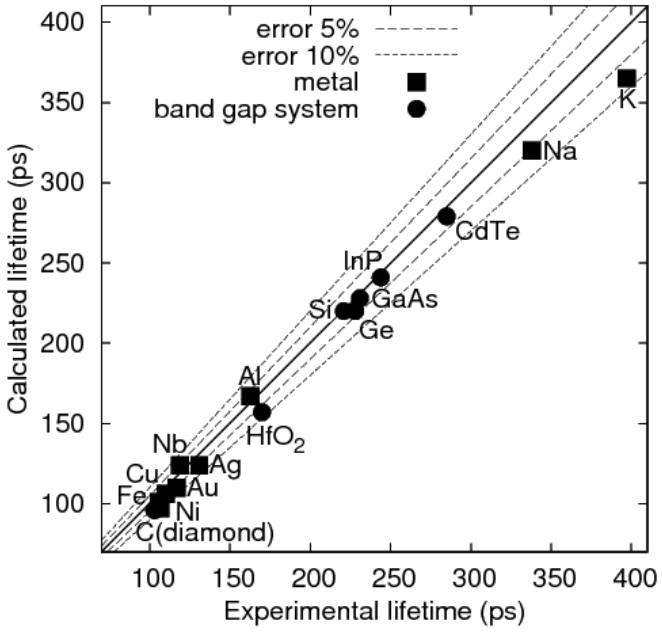

Fig. 1 Positron lifetimes.