

O44 | **Two-component density functional study of positron-vacancy interaction in metals and semiconductors**

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The positron can be utilized as a powerful probe for detecting vacancy-type defects in various solids, since positrons are selectively trapped there [1,2]. Theoretical calculations are often crucial in interpreting experimental results and in identifying defect species. To describe the positron state in solids, where many nuclei and electrons exist, Boroński and Nieminen proposed the two-component density-functional-theory formalism [3]. In many practical calculations, a simplification is made assuming that the positron affects neither the electronic structure nor the atomic arrangement. This simplified scheme is called “conventional scheme”. So far, there have been a limited number of applications of the two-component scheme in calculating positron states trapped at defects. One reason is that the computational cost for the two-component scheme is approximately 10 times higher than that for the conventional scheme. Another reason is that, in many cases, the conventional scheme and the two-component scheme give similar annihilation parameters (Doppler broadening spectra and positron lifetimes) because of the feedback effect [4]. We calculated Doppler-broadening spectra and positron lifetimes using the two schemes for divacancies in C, Si, Ge, SiC, AlN, GaN and InN and found that the difference between the two schemes depends on the bulk modulus [5]. For the relatively soft materials Si and Ge, the difference is significant.

In this study, the positron-vacancy interaction has been investigated systematically in d-block metals (except for Mn, Tc, and Hg) [6], Mg and Al as well as in III-V and II-VI semiconductors. Positron states and lifetimes for (cation) vacancies in these metals and semiconductors have been calculated by the conventional (CV) scheme and the two-component (TC) scheme with and without atomic-position relaxation. As an example of the results, the degree of atomic-position relaxation around the vacancy for metals is shown in Fig. 1.

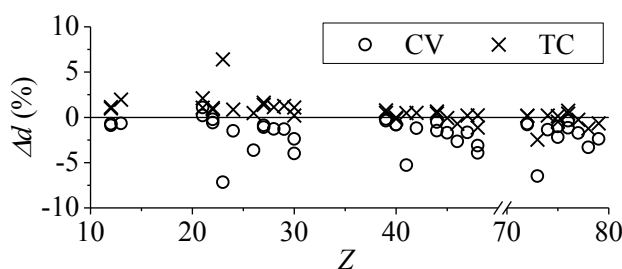


Fig.1. Z (atomic number)-dependence of the change in average distance Δd of the nearest-neighbor atoms from the vacancy center after atomic-position relaxation

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