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As_{Ga} antisite defect in GaAs

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Calculations of the electronic states associated with the As_{Ga} antisite defect in GaAs are carried out with the use of the self-consistent Green's-function technique. The defect is found to produce two deep donor levels separated by a $U \approx 0.27$ eV. The absolute positions of the levels are somewhat uncertain (~ 0.2 eV) since they are affected by corrections necessary to improve on the GaAs gap values calculated by the local-density-functional method. The overall picture, however, supports a recent experimental assignment of the As_{Ga} defect by Weber *et al.*

We present self-consistent local-density-functional (LDF) Green's-function calculations[1] of the electronic structure of the As_{Ga} antisite defect in GaAs. Two different charge states (neutral and doubly ionized defect) are studied in the ideal geometry. For both charge states, the defect induces three bound states of A_1 symmetry, one of which falls deep into the fundamental gap and is twofold occupied in the neutral state. The defect also creates a T_2 resonance above the edge of the conduction bands. Both the neutral and the doubly ionized defect give rise to very localized perturbations in the charge density of the perfect crystal. Figure 1 (bottom) shows the charge disturbance introduced by the *doubly ionized* antisite As_{Ga} defect plotted in a (110) plane. The corresponding charge profile, plotted along the [111] direction of a bond is shown in the upper panel. The dielectric screening response of the host crystal to the doubly ionized defect creates a relatively long-range charge disturbance with an integrated value of approximately $2(1-1/\epsilon)]$. The range of the corresponding neutral defect charge disturbance is considerably smaller. In Fig. 2 we show the A_1 and T_2 phase shifts. The bound states are indicated by arrows. The total charge density in the neighborhood of the *neutral* As_{Ga} defect is shown as a contour plot in Fig. 3. The As_{Ga} defect looks much like a crystal-screened arsenic atom which replaces the gallium atom. The plot also shows a double hump structure between the As_{Ga} defect and the four neighboring As atoms, similar to the bond charge shape of bulk diamond crystals.

The energy eigenvalue of the gap A_1 bound state is 1.23 eV for the neutral and 0.69 eV for the doubly ionized antisite defect (zero of energy is at the top of the valence band). A simple linear interpolation allows us to estimate U and the experimentally observable electrical levels. These are $\epsilon(++/+) = 0.83$ eV, $\epsilon(+/0) = 1.10$ eV, and $U = 0.27$ eV. The $T_2 - A_1$ splitting is 0.87 and 0.99 eV for As^0_{Ga} and As^{2+}_{Ga}, respectively. Lattice relaxation effects are not likely to be of importance in this particular case, given the comparable size of Ga and As atoms. For comparison, the recent experimental results of Weber *et al.*,[2] which have been assigned to As_{Ga} defects, are 0.52 $(++/+)$ and 0.75 eV $(+/0)$. While the theoretical

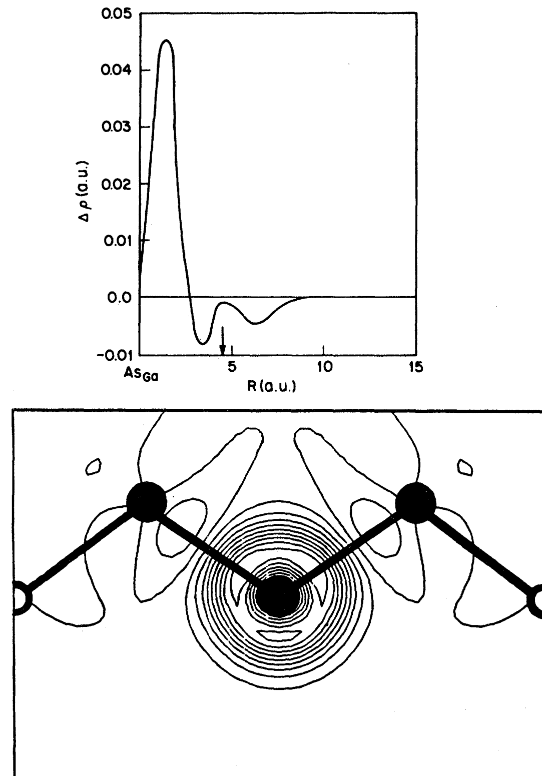

FIG. 1. Total charge disturbance introduced by As^{2+}_{Ga}, the doubly ionized arsenic antisite defect in GaAs. The contour plot (bottom) is in a (110) plane containing a GaAs bonding chain, while the charge profile (top) is taken along the [111] direction of a bond. The position of the nearest-neighbor As atom is indicated by an arrow.

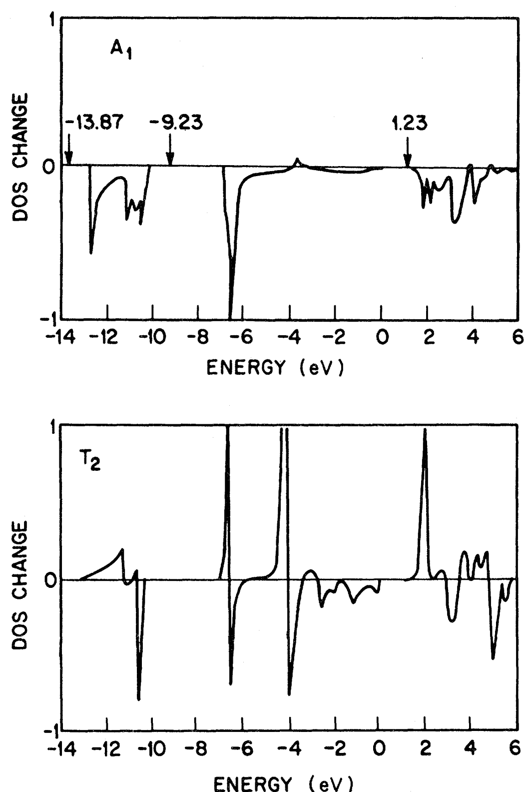

FIG. 2. Variation of A_1 and T_2 phase shifts as calculated for the neutral As_{Ga} antisite defect.

U is in excellent agreement with the measured value, the *observed* energy levels are *deeper* (by ~ 0.3 eV) than the calculated levels for As_{Ga}.

If the assignment by Weber *et al.*[2] is correct this discrepancy emphasizes an inadequacy of the LDA for the calculation of spectroscopic properties of defect systems. Straightforward use of the LDA yields a gap at Γ of ~ 0.7 eV for bulk GaAs.[3] The LDA eigenvalues have to be corrected to account for the energy- and momentum-dependent self-energy Σ for excited electrons. A first-order approximation to the effect of Σ is to assume a rigid shift of the conduction bands with respect to the valence bands. The amount of the shift can, e.g., be chosen so as to line up the experimental and theoretical conduction bands at the L point,[4] from which shallow donors in GaAs are known to derive.[5] This places the lowest conduction band at Γ considerably below the experimental value ($\Delta\epsilon = 0.28$). The band at Γ plays an almost negligible role, however, in the formation of the A_1 bound state because of the small phase space there. The value of X, which is higher than L by 0.23 eV, does influence the position of the deep donor level and is not given correctly by this rigid shift. This shows that rigid self-energy shifts of the conduction bands are not enough to correct the deficiency in LDA. In particular, an uncertainty remains in determining a conduction-band reference for the position of the energy level of the deep donor. The discrepancy of 0.3 eV between theory and experiment, which arises when the L edges are aligned, decreases to about 0.1 eV for aligned X edges. In fact, deep donorlike states derive from a large number of conduction-band states and can only approximately be associated with individual band edges. This point is demonstrated in Fig. 4 where we show the spectral distribution of the A_1 level wave function when projected onto perfect cyrstal Bloch functions. The conduction-band distribution starts at the L edge, shows a kink at the X edge, and reaches a maximum at ~ 3.0 eV where the density of states (broken line in Fig. 4) has its maximum. Numerous previous experience on defect calculations,[6] and particularly the results of Scheffler *et al.*[7] on the Ga vacancy and the antisite P_{Ga} defect in GaP, have given good evidence that similar simple procedures, adopted to overcome

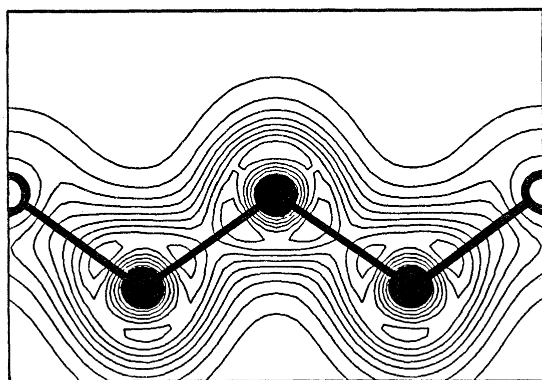

FIG. 3. Total charge density (defect plus surrounding perfect crystal) for the neutral As_{Ga} antisite defect.

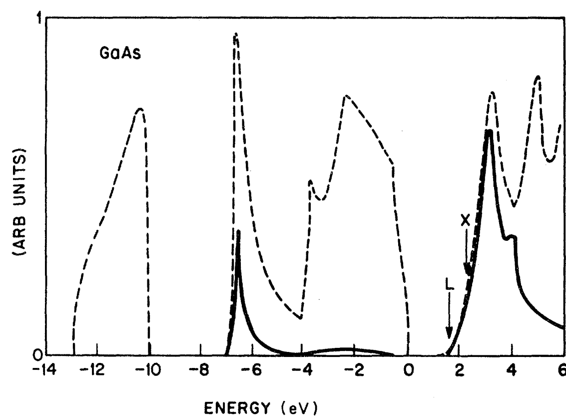

FIG. 4. Spectral distribution of the A_1 level defect wave function when projected onto crystal Bloch functions (solid line). The position of L and X conduction-band edges are indicated as well as the perfect crystal density of states (broken line).

the problems of an incorrect LDA gap, yield predictions for defect energy levels usually accurate within 0.1–0.2 eV.

In conclusion, our results predict As_{Ga} to produce two deep donor levels separated by a $U \approx 0.27$ eV which is typical for s-p materials. For the reasons we have just discussed, the absolute donor-level positions can only approximately be given. Within this uncertainty (~ 0.2 eV) the calculations support the recent assignment of the As_{Ga} defect made on the basis of photo-EPR measurements.[2]

ACKNOWLEDGMENT

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[1]For details of the method see, e.g., G. A. Baraff, E. O. Kane, and M. Schlüter, Phys. Rev. B 25, 548 (1982).

[2]E. R. Weber, H. Ennen, U. Kaufmann, J. Windscheif, J. Schneider, and T. Wosinski (unpublished).

[3]Using a converged-plane-wave basis (~ 250 waves), relativistic pseudopotentials, and Ceperley's form for exchange and correlation, we find 0.71, 1.48, and 1.15 eV for the gaps at Γ, X, and L, respectively. The defect calculations are carried out in a restricted (20 orbs/atoms) local orbitals basis, optimized to yield minimum total energy. The corresponding gaps are 0.44, 1.42, and 1.12 eV for Γ, X, and L. Thus only the value at Γ is notably affected by using the restricted local orbital basis.

[4]D. E. Aspnes, C. G. Olson, and D. W. Lynch, Phys. Rev. Lett. 37, 766 (1976).

[5]N. Lifshitz, A. Jayaraman, and M. C. Card, Phys. Rev. B 21, 670 (1980).

[6]M. Scheffler in *Festkörperprobleme,* edited by J. Treusch (Vieweg, Braunschweig, 1982), Vol. 20, p. 115.

[7]M. Scheffler, J. Bernholc, N. O. Lipari, and S. T. Pantelides, Phys. Rev. Lett. 47, 413 (1981); U. Kaufmann, J. Schneider, R. Wörner, T. A. Kennedy, and N. D. Wilsley, J. Phys. C 14, L951 (1981).