Self-consistent augmented-plane-wave band-structure calculations of Si and Ge with overlapping spheres

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We have performed self-consistent augmented-plane-wave calculations of the band structure of Si and Ge with the use of a model of overlapping muffin-tin spheres. These calculations are in good agreement with those using no shape approximation for the crystal potential.

I. INTRODUCTION

In a recent paper Glötzel, Segall, and Andersen,[1] using the self-consistent linear muffin-tin orbitals atomic-sphere approximation (LMTO-ASA) method calculated the band structure of Si, Ge, and C and obtained good agreement with calculations[2,3] that have been performed beyond the muffin-tin approximation. Glötzel *et al.*[1] also employed the idea of Keller[4] to insert empty spheres in the diamond structure and therefore increase the cell volume fraction enclosed by spheres from 0.34 to 0.68. However, since in the LMTO-ASA method the atomic polyhedra are replaced by overlapping atomic spheres, it is not clear whether the success of this approach is due to the insertion of empty spheres or to the overlapping of the spheres.

In the present work we have shown that a straightforward augmented-plane-wave (APW) calculation with overlapping muffin-tin spheres leads to results which, at least for Si, are almost identical to those of Glötzel *et al.*[1]

II. METHODOLOGY

We have used the standard APW method with spherically symmetric potentials, and with neither "warping" corrections nor "empty" spheres. We have chosen the overlapping sphere radii so as to satisfy the criterion that the fraction of the unit-cell volume inside the spheres is equal to that outside the spheres. This gives an APW sphere radius 1.137 times the radius of touching spheres. The lattice constants used in our calculations were 10.263 and 10.692 a.u. for Si and Ge, respectively. The exchange potentials have been constructed in the same manner as those of Glötzel *et al.*,[1] namely, by using the local density theory of Hedin and Lundqvist.[5] Our calculations are charge density self-consistent, again consistent with those of Glötzel *et al.*[1] The inclusion of relativistic corrections (except spin-orbit splitting) has negligible effect on Si but produces a shifting of the $\Gamma_{2'}$ state which closes the gap for Ge.

III. RESULTS AND DISCUSSION

The eigenvalues of the high-symmetry states of Si which, as we mentioned above, are not sensitive to relativistic effects, are shown in Table I where they are compared to the non-muffin-tin linear APW calculation of Hamann,[2] the linear combination of Gaussian orbitals calculations of Wang and Klein,[6] and the LMTO-ASA results.[1] We note the good agreement between the four calculations and, in particular, the close agreement between the LMTO-ASA and our calculation denoted as OAPW. The well-known conclusion that the local density theory underestimates the band gap is also observed in our calculation, as can be seen from the value 0.68 eV of the higher X_1 state which is a measure of the gap. The direct gap, given by the present calculation, is 2.76 eV at Γ, while the indirect gap in the Δ direction is 0.58 eV. It should be mentioned here that for the $\Gamma_{2'}$ state we have made the comparison with Ref. 1 in Table I using their results that include the so-called "combined correction" which attempts to correct for the overlap of the spheres. It is difficult, however, to assess this correction in our standard APW calculation.

Our energy bands for Si are plotted in Fig. 1 along the standard symmetry directions in the Brillouin zone. The bands are in excellent agreement with those obtained by Glötzel *et al.*[1] The total density of states (DOS) and its angular momentum components are plotted in Fig. 2. We note the well-known three-peak structure in the valence band, the *s* character of the low valence band, the strong *p* character of the top of the valence band and of the conduction band, and the significant *d* contribution in the conduction band.

In Table II we show our results for Ge and compare them with those of Zunger and Cohen,[3] Wang and Klein,[6] and the LMTO-ASA calculation of Glötzel *et al.*[1] For the valence band of Ge, the four calculations are in good agreement, as was the case for Si. In the conduction band, however, the states $\Gamma_{2'}$ and the higher L_1 are found significantly lower

TABLE I. Comparison of characteristic high-symmetry states in Si. The values are given in eV with respect to $\Gamma_{25'}$.

	Silicon			
	LAPW[a]	LCGO[b]	ASA[c]	OAPW[d]
Γ_1	−12.02	−12.20	−11.87	−11.87
$\Gamma_{25'}$	0.0	0.0	0.0	0.0
Γ_{15}	2.49	2.66	2.59	2.73
$\Gamma_{2'}$	3.18	3.05	3.11	2.99
X_1	−7.84	−8.03	−7.75	−7.77
X_4	−2.82	−3.11	−2.72	−2.72
X_1	0.55	0.79	0.62	0.68
$L_{2'}$	−9.64	−9.86	−9.53	−9.57
L_1	−7.06	−7.25	−6.93	−6.91
$L_{3'}$	−1.16	−1.40	−1.05	−1.16
L_1	1.40	1.46	1.57	1.36
L_3	3.37	3.66	3.51	3.55

[a]Reference 2. LAPW is linear augmented plane wave.
[b]Reference 6. LCGO is linear combination of Gaussian orbitals.
[c]Reference 1.
[d]Present calculation.

than in the other calculations and, as a result, they produce a very narrow gap. This is a nonrelativistic calculation, as are the others in Table II. We have also performed a relativistic calculation (neglecting spin-orbit splittings) following the same procedure. This calculation (as was the case in the LMTO-ASA study[1]) produces an even smaller gap at Γ due to the great sensitivity of the state $\Gamma_{2'}$. In trying to understand why our results for Si are almost identical to those of Glötzel *et al.*[1] but show significant discrepancy in the conduction band for Ge, we note that Glötzel *et al.*[1] have calculated nonrelativistic bands from their self-consistent relativistic charge densities. We have been consistent in calculating self-consistent energy bands for Ge using nonrelativistic codes for both the core charge density and the valence bands.

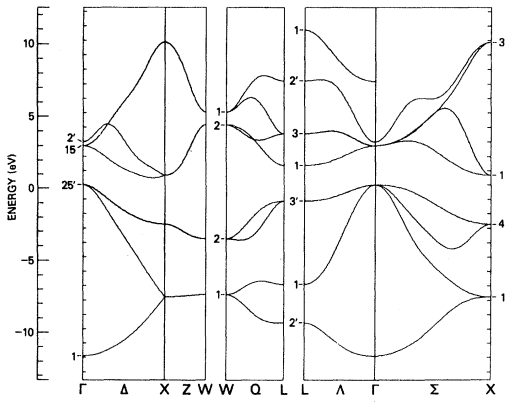

FIG. 1. Energy bands of Si.

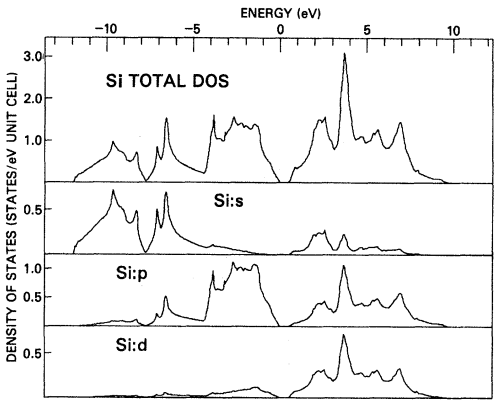

FIG. 2. Densities of states of Si.

TABLE II. Comparison of characteristic high-symmetry states in Ge. The values are given in eV with respect to $\Gamma_{25'}$.

	Germanium			
	Pseudo[a]	LCGO[b]	ASA[c]	OAPW[d]
Γ_1	−12.36	−12.46	−12.50	−12.60
$\Gamma_{25'}$	0.0	0.0	0.0	0.0
$\Gamma_{2'}$	0.77	0.72	0.59	0.26
Γ_{15}	2.59	2.61	2.59	2.76
X_1	−8.40	−8.55	−8.57	−8.71
X_4	−2.85	−3.03	−3.01	−2.93
X_1	0.95	0.88	0.64	0.76
$L_{2'}$	−10.09	−10.35	−10.33	−10.51
L_1	−7.24	−7.39	−7.46	−7.45
$L_{3'}$	−1.28	−1.40	−1.37	−1.34
L_1	0.65	0.52	0.59	0.31
L_3	3.95	3.80	3.81	3.93

[a]Reference 3. [b]Reference 6. [c]Reference 1. [d]Present calculation.

This argument, however, is weakened by the fact that the LMTO-ASA energies for $\Gamma_{2'}$ and the high L_1 are in much better agreement with the two other sets of results in Table II.

Our energy bands and DOS for Ge are shown in Figs. 3 and 4, respectively. Comparing Figs. 1 and 3, we note that our calculations give valence bands for Si and Ge which are almost identical. This is well established by the empirical pseudopotential calculations of Chelikowski and Cohen.[7] In the conduction band, Si and Ge display substantial differences. For example, at Γ the states Γ_{15} and $\Gamma_{2'}$ are interchanged. The conduction-band minimum is in the Δ direction for Si, while it is at L for Ge. Comparing Figs. 2 and 4, we observe that the total DOS as well as the angular momentum components are very similar, with the only significant difference being the smaller energy gap for Ge.

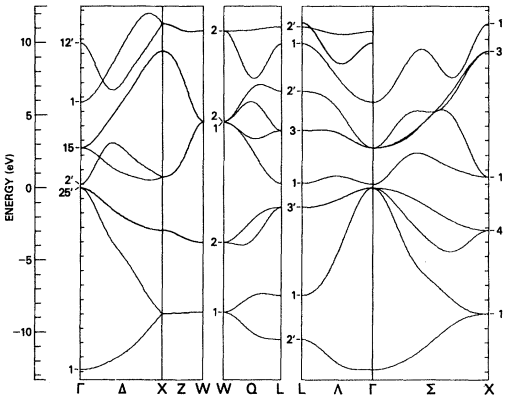

FIG. 3. Energy bands of Ge.

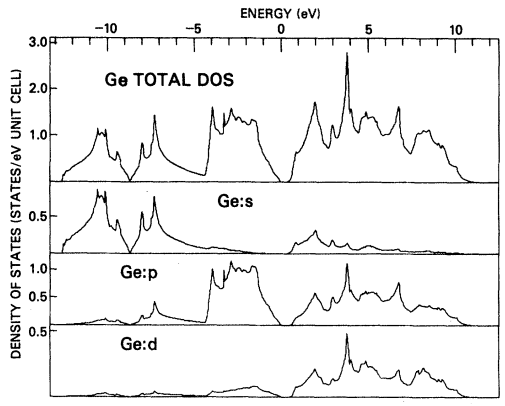

FIG. 4. Densities of states of Ge.

In a previous work[8] we had presented an APW calculation for Si in the muffin-tin approximation, without overlapping of the spheres. In that calculation, by uniformly shifting the s-like logarithmic derivatives (LD) with respect to the p- and d-like LD, we had succeeded in producing good agreement with the empirical pseudopotential results[7] in a range of 3 eV around the gap. A combination of the overlapping APW sphere method, together with the adjustment of the s-like logarithmic derivatives,[8] would give an even better agreement with experiment in the vicinity of the gap than the one we reported in Ref. 8. This sort of approach is probably a good starting point in using scattering theory to study impurities in semiconductors.

IV. CONCLUSIONS

The present calculation shows that the overlapping sphere model for Si, and to a lesser degree for Ge, gives results equivalent to calculations performed by methods which go beyond the muffin-tin approximation. The success of this method is due to the fact that we have reduced the volume of the interstitial region and hence the effect of the approximation of a constant potential in this region is minimized. In addition, the present model is also helping us in describing better the charge density. It is known[6] that the charge density reaches a maximum in the middle of the bond, therefore the overlapping spheres include more of this high charge-density volume.

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