PROCEEDINGS OF THE INTERNATIONAL CONFERENCE ON THE PHYSICS OF SEMICONDUCTORS, KYOTO, 1966
JOURNAL OF THE PHYSICAL SOCIETY OF JAPAN VOL. 21, SUPPLEMENT, 1966

I-2.

New Studies of the Band Structure of the Diamond-Type Crystals*

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By adding small empirical corrections to otherwise first-principles energy band calculations, improved energy band models have been obtained for diamond, silicon, germanium, and grey tin. These band models differ in many important respects from those derived by purely empirical (pseudopotential and full-zone $\boldsymbol{k}\cdot\boldsymbol{p}$ perturbation) methods. We have also determined how the empirical corrections required to bring first-principles band structures into agreement with experiment are affected by the inclusion of relativistic, exchange, and correlation terms.

§ 1. Introduction

Although the valence and conduction band edges** of the more important semiconductors are by now well understood, our knowledge of the band structure away from the band edges is still more qualitative than quantitative. With the rapidly expanding interest in the optical and photoemission properties of semiconductors over a broad spectral range, it is becoming increasingly important to have an accurate quantitative picture of the band structure throughout the entire reduced zone over an extended energy range (5 to 25 eV), as well as a more sophisticated qualitative understanding of the inter-relationships among the band structures of structurally and chemically related materials.

We have developed a method for determining the band structure of crystals which combines the best features of a first-principles approach[1] with the best features of an empirical approach.[2~5] Our combined or mixed approach provides a higher degree of physical insight and greater quantitative accuracy than is afforded by a purely first-principles or a purely empirical approach. In this paper we will discuss the essential features of our method, as well as applications to the diamond-type crystals. Our present results for silicon, germanium, and grey tin are compared with experiment and with theoretical results obtained by other methods in a forthcoming paper[6] which should be read in conjunction with this one. We are currently investigating the band structures of several sphalerite- and wurtzite-type crystals by the present method, and we hope to report our results for these crystals in the near future.

§ 2. Theoretical Considerations

Our starting point is a non-relativistic self-consistent (NRSC) energy band calculation based on Slater's free-electron exchange approximation.[1] The essential innovation in the present work is the introduction of an empirical crystal potential correction ΔV which hopefully compensates for our simplified treatment of exchange, and for our neglect of relativistic and correlation (many-electron) effects. This correction is determined by adjusting relevant features of the theoretical band structure to the most firmly established experimental features, typically the direct and indirect band gaps. It is noteworthy that the empirical correction required to bring theory into agreement with experiment is usually quite small. In grey tin, for example, the empirical correction amounts to changing three of the leading Fourier coefficients of the NRSC crystal potential by 0.5, 1, and 2 percent. The empirical correction can be reduced by modifying

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* The research reported in this paper was sponsored in part by the Lockheed Independent Research Fund; the Air Force Cambridge Research Laboratories, Office of Aerospace Research, under Contract No. AF 19(628)-5750: and the Aerospace Research Laboratories, Office of Aerospace Research, under Contract No. AF 33(615)-5072.

** By *band edges* we mean the highest valence band maximum and the lowest conduction band minimum, as well as subsidiary conduction band minima, such as the (000) and (100) minima in germanium.

the underlying physical model, but the correction is already so small for our simplified model that it is not really essential to devote additional effort attempting to refine the physical model, at least in such favorable cases as grey tin.

Let us now introduce our notation. We will denote the first-principles (NRSC) energy band structure by E(NRSC), and the empirically corrected (or perturbed) theoretical band structure by E(PERT), where $E(\mathrm{PERT})=E(\mathrm{NRSC})+\Delta E(\Delta V)$. Here $\Delta E(\Delta V)$ denotes the energy level shifts induced by ΔV. Note that ΔV is a correction to our NRSC crystal potential, rather than a pseudopotential. Let the (actual) experimental band structure be denoted by E(EXPT), and the experimental band structure with the spin-orbit splitting removed by E^*(EXPT), where $E^*(\mathrm{EXPT})=E(\mathrm{EXPT})-\Delta E(\mathrm{SO})$. Each energy level in E^*(EXPT) is defined as the weighted mean of the corresponding spin-orbit split levels in E(EXPT). In the present work, experimental values are used for the energy level shifts induced by spin-orbit interaction, ΔE(SO). In future work, we hope to supplement experimentally known values of ΔE(SO) by values obtained from first-principles calculations.

In practice, ΔV is expressed in terms of a limited number of adjustable parameters[†], and the energy level shifts $\Delta E(\Delta V)$ are determined by first-order perturbation theory; this procedure is usually justified because ΔV proves to be quite small. The next step is to adjust $E(\mathrm{PERT})=E(\mathrm{NRSC})+\Delta E(\Delta V)$ to the most firmly established features (interband transition energies) of E^*(EXPT), by suitably choosing the adjustable parameters appearing in ΔV. It is necessary to determine the sensitivity of the adjusted solution, E(PERT), to variations in the choice of ΔV, since the empirical adjustment can usually be carried out satisfactorily in a wide variety of ways.

Fortunately, many features of E(PERT) prove to be relatively insensitive not only to the exact choice of ΔV, but also to the exact choice of the physical model underlying the NRSC band calculation.[6)] The uncertainties in E(PERT) can be minimized by adjusting the most "sensitive" features of E(PERT) to experiment, rather than the least "sensitive." When this cannot be done, *i.e.*, when the most "sensitive" features are not known experimentally, these features in E(PERT) remain somewhat uncertain, but our approach does at least provide some measure of this uncertainty, which is often quite helpful.

By making a systematic study of the different types of $\Delta E(\Delta V)$ induced by different types of ΔV, we have been able to demonstrate[6)] that there are in fact a rather limited number of energy level shift patterns $\Delta E(\Delta V)$, in spite of the wide variations possible in the choice of ΔV. In the case of the diamond-type crystals, for example, there are only three distinctive $\Delta E(\Delta V)$ patterns of practical interest. The foregoing analysis provides a rational basis for constructing an extremely flexible adjustment scheme in terms of a minimum number of parameters. At the same time, the amount of experimental information required for fitting E(PERT) to E^*(EXPT) can be greatly reduced, which is an important practical advantage.

§ 3. Grey Tin

We will now illustrate our approach by considering a three-parameter E(PERT) energy band model for grey tin based on the parameters $\Delta v(111)$, $\Delta v(220)$ and $\Delta v(311)$, which generate the three different $\Delta E(\Delta V)$ patterns alluded to above. We will remove two of the three degrees of freedom from E(PERT) by adjusting E(PERT) to the experimental values [E^*(EXPT)] of the direct [000] and indirect [111] band gaps given by the analysis of Groves and Paul,[6,7)] namely, $\Gamma_{2'}-\Gamma_{25'}=-0.16$ eV, and $L_1-\Gamma_{25'}=0.32$ eV. Selected features of E(PERT) are plotted in Fig. 1 as a function of the sole remaining degree of freedom, which we arbitrarily represent by $\Gamma_{15}-\Gamma_{25'}$.

Since one of our principal objectives is to confirm or contradict current interpretations of reflectivity and electroreflectivity spectra which identify characteristic spectral structure with specific interband transitions, we will not use such interpretations (in an important way) in constructing our E(PERT) model. Actually, many of these interpretations are not particularly helpful because spectral structure of known energy is assigned to (critical-point) transitions which cannot be located accurately in the reduced zone.

Accordingly, we will back off one step, and construct a number of two-parameter E(PERT)

[†] It is convenient to express ΔV as a Fourier series, and to treat the Fourier coefficients, $\Delta v(\boldsymbol{h})$, as adjustable parameters. It is usually sufficient to include only the leading Fourier coefficients of ΔV, for example, $\Delta v(111)$, $\Delta v(220)$, and $\Delta v(311)$. See ref. 6) for further details.

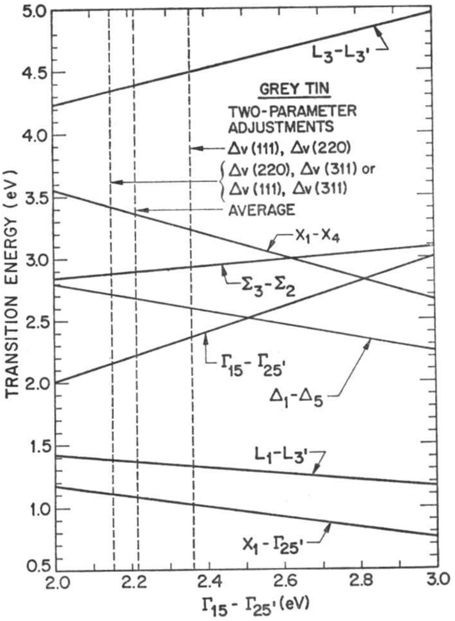

Fig. 1. Selected transition energies in grey tin vs. $\Gamma_{15}-\Gamma_{25'}$, according to a three-parameter E(PERT) model which has been adjusted to the experimental direct and indirect band gaps, and hence has only one degree of freedom left. The Δ and Σ transitions refer to the zone points $(2\pi/a)(1/2\,0\,0)$ and $(2\pi/a)(1/2\ 1/2\,0)$.

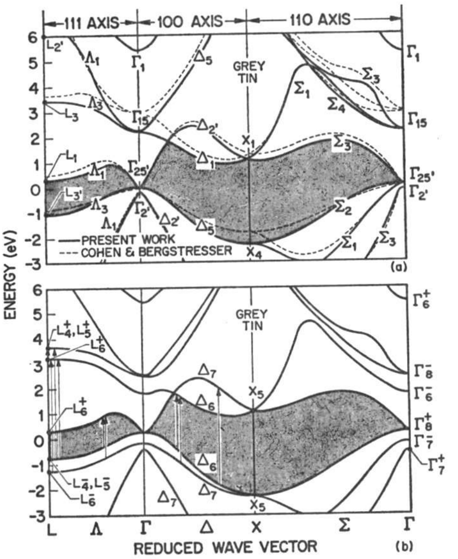

Fig. 2. Energy band structure of grey tin, with the spin-orbit splitting omitted in (a) and included in (b). Critical-point transitions that might account for the spectral structure observed in electroreflectance by Cardona *et al.*[8] are indicated by vertical arrows in (b). The transitions shown along the [111] axis and at L are the same as those proposed by these authors, while those shown along the [100] axis are somewhat different.

solutions, each of which is required to reproduce the experimental direct and indirect band gaps, which are the only two well-established features of the experimental band structure (in our opinion). These special cases are indicated in Fig. 1 by vertical dashed lines. It is noteworthy that the three different two-parameter E(PERT) solutions all fall so close together; in fact, two of them are nearly coincident and hence are indicated by the same vertical dashed line. Encouraged by this small dispersion of the individual two-parameter solutions, we will adopt as our E(PERT) model the arithmetic average of the two-parameter solutions, which is also shown in Fig. 1. Of course, this model is adopted on a provisional basis, subject to experimental confirmation.

Our provisional E(PERT) model is displayed in greater detail in Fig. 2(a), together with the three-parameter pseudopotential band model of Cohen and Bergstresser[3] (hereafter CB), which is based on the pseudopotential counterparts of our $\Delta v(111)$, $\Delta v(220)$ and $\Delta v(311)$. Considering the radically different methods used by CB and ourselves in arriving at the band models in Fig. 2(a), the agreement is quite remarkable. However, one must not overlook the serious discrepancy in the neighborhood of the triply-degenerate conduction band state Γ_{15}; a similar discrepancy shows up, incidentally, in germanium and silicon. For grey tin, our value of $\Gamma_{15}-\Gamma_{25'}$ is 2.2 ± 0.15 eV, which is significantly less than CB's value of 3.0 eV.

It is clear from Fig. 1 that we can push $\Gamma_{15}-\Gamma_{25'}$ up to 3.0 eV within the framework of our general three-parameter E(PERT) band model, but this leads to unreasonably low values for X_1-X_4 and unreasonably high values for $L_3-L_{3'}$, if we are to judge by the analogous situations in germanium and silicon.[6] For example, in these two crystals, our E(PERT) values for X_1-X_4 are 4.1 ± 0.1 eV, and the main reflectivity peak falls at 4.5 eV. In grey tin, our E(PERT) value for X_1-X_4 is 3.4 ± 0.1 eV, and the corresponding reflectivity peak[9] falls at 3.65 eV. If we were to set $\Gamma_{15}-\Gamma_{25'}$ to 3.0 eV in grey tin (CB's value), we would find (cf. Fig. 1) that X_1-X_4 falls to 2.65 eV, a full eV below the 3.65 eV reflectivity peak to which it is most probably related. As is explained more fully elsewhere,[6] we believe that our *E*(PERT) model for grey tin is more accurate than CB's.

Our estimate of the band structure of grey tin with the spin-orbit splitting taken into account is sketched in Fig. 2(b). (The splitting shown here is based on our best current estimates, and not on actual first-principles $\Delta E(\Delta V)$ values.) Our spin-orbit split band model for grey tin [Fig. 2(b)] differs from Cardona *et al.*'s[8] to about the same extent that our unsplit band model [Fig. 2(a)] differs from CB's. In both cases the principal discrepancy is at Γ_{15}.

§ 4. Germanium and Silicon

Proceeding along similar lines, we have obtained *E*(PERT) band models for germanium and silicon which are qualitatively similar to recently proposed empirical band models[2~5] but quantitatively different in a number of important respects.[6] We have also determined the deformation potentials for important interband transitions in germanium and silicon, as well as the changes in the band structure of germanium produced by major changes in the lattice constant. All of these new results are reported in detail and compared with experiment and with other theoretical results elsewhere.[6] Because of space limitations, we will confine ourselves here to a pictorial comparison between our *E*(PERT) band models and CB's pseudopotential band models (cf. Figs. 3 and 4), and to a few brief remarks.

As can be seen from Figs. 2, 3 and 4, our calculated values for $\Gamma_{15}-\Gamma_{25'}$ are consistently lower than CB's by at least 0.5 eV. Since CB's values reflect current interpretations of optical and photoemission spectra, the systematic discrepancy between our $\Gamma_{15}-\Gamma_{25'}$ values and CB's leads us to question the correctness of these interpretations. Our results suggest that the $\Gamma_{15}-\Gamma_{25'}$ transition has not been properly identified in previous work.[10] A downward revision in $\Gamma_{15}-\Gamma_{25'}$ by even 0.5 eV would have a profound effect on the structure of three of the four lowest conduction bands in the central region of the reduced zone, and on the detailed nature of interband transitions in the range between 2 and 4 eV.

Since rather strong claims have been made[2,3,10] about the accuracy of the empirical pseudopotential method (EPM), it is noteworthy that our independent approach leads to band structures that are significantly different from the pseudopotential band structures in certain important respects. (Surely the 0.8 ± 0.15 eV discrepancy at Γ_{15} in grey tin is an "important" and "significant" discrepancy.) Such large discrepancies are not expected to arise in well-understood regions of the band structure, since the pseudopotential band structures and our own have both been adjusted to agree with experiment in such regions. The real test of the EPM is its ability to predict accurately the nature of the band structure in presently unknown or poorly understood regions. The same remark applies to our own method, of course. Although Cohen and Bergstresser[3] claim that their pseudopotential band structures are consistent with experiment to within about 0.15 eV near the forbidden band, and to within about 0.5 eV over

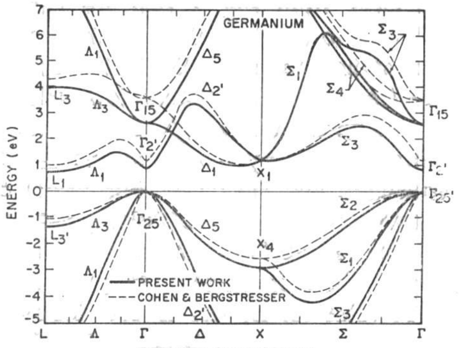

Fig. 3. Comparison of two energy band models for germanium. Our *E*(PERT) solution has been adjusted only to the experimental direct [000] and indirect [111] band gaps. See ref. 6) for further details.

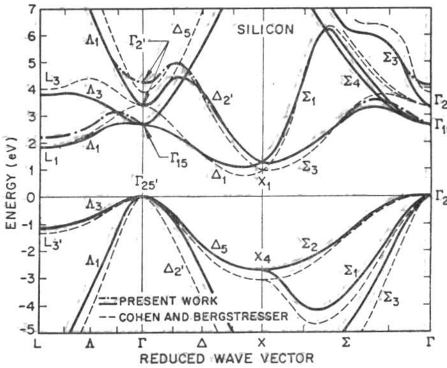

Fig. 4. Comparison of three energy band models for silicon. Both *E*(PERT) solutions have been adjusted to the experimental indirect [100] band gap, but to different assumed values for $L_1-L_{3'}$. See ref. 6) for further details.

a 15 eV energy range, our independent studies suggest that these estimates are somewhat optimistic. We believe that the pseudopotential band structures may deviate from experiment by as much as 0.5 to 1.0 eV in certain regions. On the whole, we regard the work of Cohen and Bergstresser as a major step forward, and we hope that current discrepancies between their work and our own will soon be resolved (by experiment).

§ 5. Diamond

While the differences between pseudopotential band models and our *E*(PERT) band models are usually less than 1 eV in grey tin, germanium, and silicon, the differences are considerably greater in diamond (cf. Fig. 5). The *E*(PERT) model shown has been adjusted to the experimental indirect band gap, $\Delta_1{}^m - \Gamma_{25'} = 5.47$ eV. The conduction band minimum, $\Delta_1{}^m$, falls 3/4 of the way from Γ to X, which is in accord with experiment. Our *E*(PERT) model pins down the insensitive transition energies ($\Gamma_{15}-\Gamma_{25'}$, X_1-X_4, $L_3-L_{3'}$) to within a few tenths of an eV, but the sensitive transition energies ($\Gamma_{2'}-\Gamma_{25'}$, $L_1-\Gamma_{25'}$) are not pinned down nearly this well.

However, even if we take the uncertainties in our *E*(PERT) solution into account, this solution is profoundly different from the pseudopotential solution of Saslow, Bergstresser, and Cohen[11] (hereafter SBC), except in the neighborhood of the band edges, to which both solutions have been adjusted. When we *predicted* the nature of the conduction band edge in diamond in 1952,[12] little did we dream that the remainder of the band structure would still contain elements of controversy 14 years later!

Apart from the 1 to 3 eV discrepancies in the neighborhood of the forbidden band, we call attention to the 10 eV discrepancy in the location of the 3d-like conduction band state $\Gamma_{12'}$, and to the 7 eV discrepancy in the location of the lowest valence band state (Γ_1). It is clear from Fig. 5 that all of these discrepancies are systematically related, and that the large discrepancies far away from the forbidden band are still felt, though in attenuated form, in the physically important region bordering the forbidden band.

In view of the discrepancies between our *E*(PERT) model for diamond and SBC's pseudopotential band model, the detailed nature of the conduction bands away from the band edge must be regarded as an open question. We cannot accept many of SBC's interpretation of the ex-

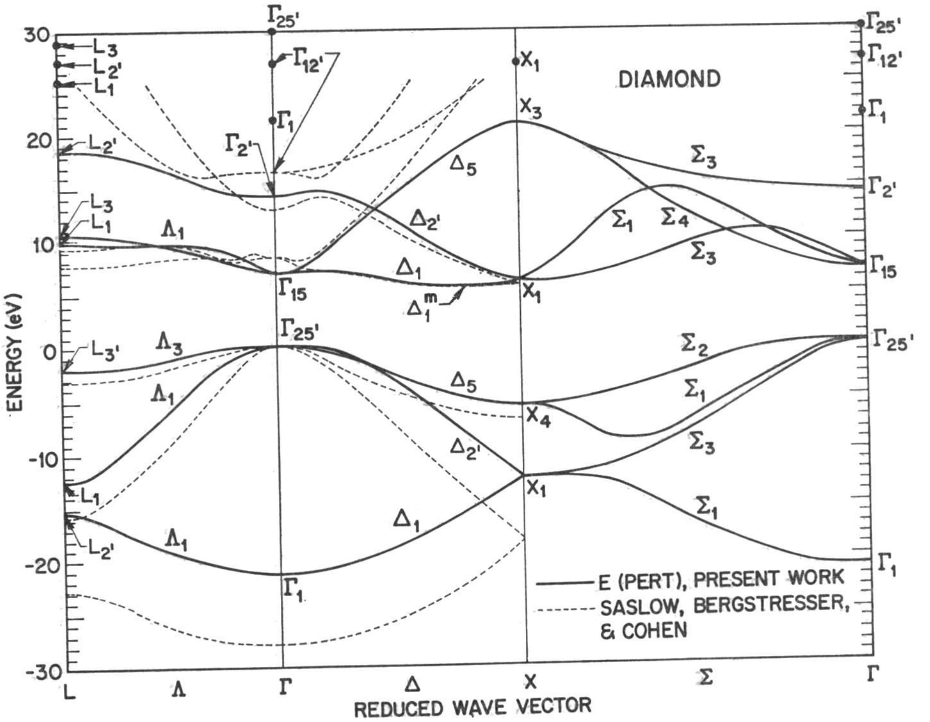

Fig. 5. Comparison of two energy band models for diamond.

perimental reflectivity spectrum of diamond, partly because these interpretations are based on experimental data that have since been modified by more careful work[13)], and partly because SBC's pseudopotential band model is of doubtful accuracy, at least away from the valence and conduction band edges.

Of all the crystals that have been studied thus far by the empirical pseudopotential method (and by our own method), diamond has proved to be the most difficult crystal to handle theoretically. In our opinion, SBC's pseudopotential band model for diamond is the least accurate of all the pseudopotential band models published thus far. Of all our E(PERT) models, that for diamond is most uncertain. However, the uncertainties in our E(PERT) model for diamond represent only a small fraction of the differences between this model and SBC's pseudopotential band model.

Recent experimental measurements[13)], our recent theoretical studies, and even SBC's theoretical studies all cast serious doubt on Phillips' estimate[10,14)] that $\Gamma_{15}-\Gamma_{25'}$ in diamond is about 8.7 eV. (The correct value is more nearly 7.0 eV.) Further theoretical and experimental studies of the band structure of diamond are clearly in order.

§ 6. Discussion

The present approach to band structure calculations was developed for three principal reasons. First, we recognized that some form of empirical correction was necessary if the difficulties involved in treating exchange, correlation, and relativistic effects rigorously were to be circumvented.

Second, we recognized that purely empirical (pseudopotential and full-zone $\boldsymbol{k}\cdot\boldsymbol{p}$ perturbation) methods were not nearly as accurate as some of their advocates would have us believe, and that it would be far better to add a small empirical correction to a physically reliable first-principles band calculation than to depend entirely on the caprices of fully empirical adjustments. By fitting our theoretical band models only to well-established experimental information, thereby freeing ourselves from previous speculations[10)] concerning the nature of the band structure away from the band edges, we have been able to take a fresh look at the entire band structure, including such poorly understood regions as the conduction band structure associated with the triply-degenerate state Γ_{15}. It is noteworthy that the major discrepancies between our band models and those derived by purely empirical methods occur in the neighborhood of Γ_{15} (in silicon, germanium, and grey tin). By calling attention to these discrepancies, we hope to stimulate further theoretical and experimental studies of the band structure of these crystals, particularly in the vicinity of Γ_{15}.

Third, and perhaps most important of all from a long range point of view, we recognized that the small empirical correction ΔV required to bring our first-principles theory into agreement with experiment could be used as a guide in the progressive improvement of this first-principles theory, and in the progressive reduction in the magnitude of ΔV. We have already learned the following important lessons:

(a) If the relativistic (mass-velocity and Darwin) corrections ΔE(REL) are included by first-order perturbation theory, so that $E(\mathrm{PERT}) = E(\mathrm{NRSC})+\Delta E(\Delta V)$ is replaced by $E(\mathrm{PERT})= E(\mathrm{NRSC})+\Delta E(\mathrm{REL})+\Delta E(\Delta V')$, $\Delta V'$ is usually larger than ΔV, which means that $E(\mathrm{NRSC})+\Delta E(\mathrm{REL})$ is actually further removed from experiment [E^*(EXPT)] than is E(NRSC).

(b) If the E(NRSC) band calculation is "improved" by replacing Slater's free-electron exchange approximation by Slater's averaged Hartree-Fock exchange approximation,[15,1)] the agreement between E(NRSC) and E^*(EXPT) is worsened. By extension, we would expect a rigorous Hartree-Fock NRSC band structure to depart even further from experiment.

(c) On the other hand, if we screen Slater's free-electron exchange approximation, the agreement between E(NRSC) and E^*(EXPT) can be improved. If the relativistic corrections are not included, a weak screening of the exchange term is sufficient, while if the relativistic corrections are included, a stronger screening of the exchange term is required to improve the agreement between theory and experiment.

(d) Let us denote by ΔE(EXCH) the energy level shifts introduced by screening the exchange terms, and let us include the relativistic corrections in our E(PERT) scheme, so that we have: $E(\mathrm{PERT}) = E(\mathrm{NRSC}) + \Delta E(\mathrm{EXCH}) + \Delta E(\mathrm{REL})+ \Delta E(\Delta V'')$. Our general experience is that ΔE(EXCH) counteracts ΔE(REL), and that $\Delta V''$ can be made considerably smaller than our original ΔV by screening the exchange term in a suitable manner. The closer the exchange term used in the NRSC band calculation is to the rigorous Hartree-Fock exchange term, the stronger must the exchange screening be to minimize the value of $\Delta V''$.

The good qualitative agreement between experiment and E(NRSC) based on Slater's free-electron exchange approximation appears to be partly accidental, arising from the partial compensation of neglected relativistic terms by neglected exchange and correlation terms. In order to develop a more satisfactory first-principles theory, it is not sufficient merely to improve the treatment of relativistic effects, just as it is not sufficient merely to improve the treatment of exchange and correlation effects. Since these two refinements tend to have opposite effects on the band structure (in the cases we have studied), they should be incorporated simultaneously in any future theory.

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DISCUSSION

Reiss, H.: I take it that you no longer think that relativistic effects to be important.

Herman, F.: Relativistic corrections are in fact very important in crystals such as silicon and germanium. However, in our present approach, these corrections do not have to be treated explicitly, but can be included in that empirical correction $\Delta E(\Delta V)$. This point is discussed further in the text of our paper.

Cohen, M. L.: It is gratifying that adjusted OPW calculations and pseudopotential calculations agree so well. The main disagreement is the Γ_{15} level in Si, Ge and Sn, and this disagreement can only be settled by experiment.

The important thing that theorists should focus on is the similarity of the band structures. Our pseudopotential calculations involve local, k-independent, E-independent potentials, and these potentials appear to give correct band structures, *i.e.* agreement with experiment is excellent. It seems that there is a very general cancellation theorem at work here. Perhaps the theorem is similar to the original Phillips' cancellation which shows that a weak pseudopotential is valid, and one can show generally that a k-independent, slightly E-dependent pseudopotential is a very good representation for a crystal potential.

Herman, F.: The statement by Cohen that "pseudopotential band calculations appear to give correct band structures because the agreement between theory and experiment is excellent" is somewhat misleading. It must be borne in mind that in most cases pseudopotential band structures are deliberately adjusted to "experiment" so that the agreement between "theory" and "experiment" is largely a confirmation of the success of the empirical fit. There is always the possibility that "theory" has been fitted to misinterpreted or incorrect experimental information. We believe that the pseudopotential band structures for silicon, germanium, and grey tin have been fitted to misinterpreted experimental information in the neighborhood of the Γ_{15} conduction band level, and that this circumstance accounts, at least in part, for the important differences between the pseudopotential band structures and our own in the neighborhood of this level. The principal danger of the pseudopotential approach is that "theory" can bias interpretation of experiment, and vice versa. (Our own approach is less susceptible to such bias because we are less dependent on theoretical interpretations of imprecise experimental data than are the pseudopotential people.) Clearly, some independent assessments of the experimental situation are in order.

Even when the experimental data have been correctly interpreted, pseudopotential band structures often fail to reproduce the experimental band structures by a few tenths of an eV. We would not be surprised if subsequent experimental work shows pseudopotential band structures to be in error by 0.5 to 1.0 eV in unadjusted regions of the band structure, in an energy range not too far removed from the forbidden band.

I think it is wonderful that pseudopotential band calculations and our present band calculations are in such good qualitative agreement, not only with one another, but with energy band pictures (for germanium and silicon) published by ourselves and others over a decade ago.