PHYSICAL REVIEW B VOLUME 10, NUMBER 4 15 AUGUST 1974

Pressure dependence of energy gaps and refractive indices of tetrahedrally bonded semiconductors

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(Received 1 October 1973; revised manuscript received 8 April 1974)

The pressure dependence of energy gaps for a number of elemental and compound semiconductors is investigated employing the empirical pseudopotential method. The compressibility and the empirical pseudopotential form factors appropriate for describing the band structure at normal pressure are the only required input parameters in this calculation. The calculated pressure coefficients of several critical-point band gaps for group IV and III-V compounds are generally in good agreement with experimental data. The results are then utilized, along with a Penn type of single-oscillator model for the dielectric constant, to calculate the pressure coefficient of the refractive index. The results are good for elemental semiconductors and reasonable for III-V compounds. Similar calculations of pressure coefficients of both the energy gaps and the refractive index for several II-VI compounds yield results which are less satisfactory. Possible reasons for this discrepancy are discussed.

I. INTRODUCTION

Many experiments[1-3] have been performed to determine the pressure coefficients of various energy gaps and/or optical transition energies in semiconductors. The general results indicate that the symmetries of the initial and the final states involved in an optical transition play an important role in determining the pressure dependence of that energy gap. Theoretical calculations, on the other hand, are relatively limited. Herman *et al.*[4] calculated the pressure coefficients of several band gaps for Si and Ge using a self-consistent orthogonalized-plane-wave (OPW) method. Goroff and Kleinman[5] have calculated, also by the OPW method, the volume-deformation potentials for selected band gaps of Si. Brust and Liu[6] have calculated the high-pressure band structure of Si and Ge. The pressure derivatives of the pseudopotential form factors required in their calculation were determined empirically by fitting the calculated pressure coefficients of certain critical-point band gaps to experimental values. Recently, Melz[7] performed a calculation for some elemental and III-V semiconductors, where the change in pseudopotential form factors due to pressure was obtained from the general shape, in reciprocal space, of the Heine-Abarenkov model potential.[8] The OPW calculations are, in general, rather cumbersome to perform, and are not easily extendable to the case of compound semiconductors. The empirical approach of Brust and Liu is unsatisfactory in that it requires fitting pressure coefficients of some band gaps to experimental data in order to determine changes of form factors with pressure; thus, it is less desirable as a predictive method. Furthermore, an extension of the method to compound crystals is highly unpracticable, because in the latter case, aside from the three symmetric form factors required for elemental semiconductors, one also has three antisymmetric form factors whose pressure derivatives must also be fitted. Melz's calculation, on the other hand, is relatively straightforward. However, in addition to requiring the empirical pseudopotential form factors, which yield satisfactory band structures at atmospheric pressure, it also relies on the Heine-Abarenkov model potential for determining the wave-vector (q) dependence of the pseudopotential form factors. The results obtained for several III-V compound semiconductors were only within about a factor of 2 of experimental values.

In this work, we first present a simpler scheme for calculating the pressure dependence of critical-point energy gaps for a number of elemental and compound semiconductors. We use as input data, only the compressibility and the empirical pseudopotential form factors (PFF's) appropriate for band structure at normal pressure. In contrast to Melz's calculation, no model potentials are used to determine the q dependence of the PFF's; instead, these are established numerically. With a few exceptions, our calculated pressure coefficients of several important band gaps are, in general, within 25% or so of experimental results; and the good agreement is rather uniform for group IV as well as III-V compounds, in contrast with the results of Melz, where it was found that the agreement became worse going from elemental to compound crystals. Encouraged by this improvement, we next present a calculation of the pressure dependence of refractive indices of these crystals,

using a single-oscillator model. The calculated values of dn/dp generally agree fairly well with available experimental data, as well as with results determined semiempirically from an extension[9] of Van Vechten's dielectric theory in the case of elemental and III-V semiconductors. Results of similar calculations for II-VI compounds are less satisfactory. Possible reasons for this discrepancy are discussed.

II. METHOD OF CALCULATION

The pseudopotential-energy-band calculation[10] involves the solution of the wave equation with a crystal pseudopotential $V(\vec{r})$, which is much weaker than the real potential and is normally taken as the superposition of atomic (or ionic) pseudopotentials. For crystals of interest here, $V(\vec{r})$ can be conveniently written

$$V(\vec{r}) = \sum_{\vec{G}} [V^s(\vec{G})\cos(\vec{G}\cdot\vec{\tau}) + iV^A(\vec{G})\sin(\vec{G}\cdot\vec{\tau})]\, e^{i\vec{G}\cdot\vec{r}}, \quad (1)$$

where

$$V^s(\vec{G}) = V_1(\vec{G}) + V_2(\vec{G}), \quad V^A(\vec{G}) = V_1(\vec{G}) - V_a(\vec{G}),$$

and $\vec{\tau} = \frac{1}{8}a(1,1,1)$, where a is the lattice constant and $\vec{G}$ is a reciprocal lattice vector. $V_i(\vec{G})$, where $i = 1$ or 2, is the atomic PFF obtained from $V_i(\vec{q})$, the Fourier transform of the ith screened ionic pseudopotential, for $\vec{q} = \vec{G}$. The latter can be formally written[10]

$$V_i(\vec{q}) = \frac{1}{\Omega\epsilon(\vec{q})} \int V_i(\vec{r})\, e^{-i\vec{q}\cdot\vec{r}}\, d\vec{r}. \quad (2)$$

In Eq. (2), $\Omega(=\frac{1}{4}a^3)$ is the primitive cell volume; $\epsilon(\vec{q})$ is the wave-vector-dependent dielectric function,[11] which accounts for the screening effect of the valence electrons; and $V_i(\vec{r})$ is the ionic pseudopotential of the ith ion. Equation (2) provides a prescription for calculating band structure of a crystal at a higher pressure.

If no phase transition occurs, then the effects of pressure on the crystal band structure will arise, essentially, from just the change in lattice constant. From Eq. (2), it is obvious that $V_i(\vec{q})$ is affected by the lattice constant through the cell volume Ω, the dielectric function ϵ, and the reciprocal lattice vector $\vec{G}$, and possibly also through the dependence of $V_i(\vec{r})$ on the lattice constant. In the present work, however, we adopt the rigid-ion approximation,[5] where $V_i(\vec{r})$ remains unchanged for small variations (of the order of a few percent) of the lattice constant. Similar assumptions were also made in previous works.[5–7,12] It follows that

$$U_i(\vec{q}) \equiv \int V_i(\vec{r})\, e^{-i\vec{q}\cdot\vec{r}} d\vec{r} = V_i(\vec{q})\Omega\epsilon(\vec{q}) \quad (3)$$

will not depend explicitly on the lattice constant (the implicit dependence arises through $\vec{q}$). The same statement holds true for

$$U^{S,A}(\vec{q}) \equiv V^{S,A}(\vec{q})\Omega\epsilon(\vec{q}). \quad (4)$$

To calculate the band structure at a higher pressure, one needs the symmetric and antisymmetric PFF's at pressure p,

$$V_p^S(\vec{G}_p), \quad \text{for } \vec{G}_p = (\sqrt{3}, \sqrt{8}, \sqrt{11})2\pi/a_p,$$

and

$$V_p^A(\vec{G}_p), \quad \text{for } \vec{G}_p = (\sqrt{3}, 2, \sqrt{11})2\pi/a_p,$$

where the subscript p refers to quantities at pressure p. V_p^S and V_p^A are now given by

$$V_p^{S,A}(\vec{G}_p) = U^{S,A}(\vec{G}_p)/\Omega_p\epsilon_p(\vec{G}_p), \quad (5)$$

so that values of $U^{S,A}(\vec{G}_p)$ are required. These can be readily obtained if the $\vec{q}$ dependence of $U^{S,A}(\vec{q})$ are known.

In principle, one can establish the $\vec{q}$ dependences of $U^{S,A}(\vec{q})$ by making use of analytical expressions[10] derived from certain model potentials, along with an appropriate $\epsilon(\vec{q})$. However, since most model potentials are based on drastic and/or unphysical assumptions, it is felt that the $\vec{q}$ dependence established from them may be inadequate for the present purpose; this was partially reflected in the results of Melz's calculation, where one of the most carefully constructed model potentials, namely, the Heine-Abarenkov model potential, was employed.

In the present investigation, we find that better results are obtained by simply fitting polynomials to each set of empirical values of $U^S(\vec{G})$ and $U^A(\vec{G})$, thereby establishing their respective $\vec{q}$ dependences. The values of $U^S(\vec{G}_p)$ and $U^A(\vec{G}_p)$ needed for high-pressure calculations, then, are readily obtainable from these polynomials.

Next the dielectric function $\epsilon(\vec{q})$ and its pressure dependence have to be determined. Several calculations of $\epsilon(\vec{q})$ based on realistic band-structure models have been reported.[13] However, they are invariably presented in numerical forms from which it is impossible to deduce the pressure dependence of $\epsilon(\vec{q})$. To get around this difficulty, we make use of a model dielectric function $\epsilon^*(\vec{q})$ first derived by Penn[14] and subsequently modified by Brust,[15] namely,

$$\epsilon^*(\vec{q}) = 1 + 0.65[\epsilon(\vec{q}) - 1][1 - f_H(\vec{q})],$$

where

$$\epsilon(\vec{q}) = 1 + (\hbar\omega_p/E_g)^2 F[1 + (E_F/E_g)(q/K_F)^2 F^{1/2}]^{-2}$$

and

$$F = 1 - 0.25(E_g/E_F).$$

ω_p, E_F, and K_F are, respectively, the plasma frequency, Fermi energy, and Fermi wave vector corresponding to the appropriate valence-electron

TABLE I. Pressure coefficients of important band gaps[a] (in 10^{-6} eV bar^{-1}).

	$\frac{dE_0}{dp}$		$\frac{dE_1}{dp}$		$\frac{dE_x}{dp}$		$\frac{dE_{\Gamma L}}{dp}$		$\frac{dE_{\Gamma x}}{dp}$	
	Calc.	Expt.	Calc.	Expt.	Calc.	Expt.	Calc.	Expt.	Calc.	Expt.
Si	1.3	1 ± 1[b]	6.6	6.2 ± 0.4[b]	3.6	3	5.5	...	$0.5\sim-0.1$	−1.5
Ge	16.2	14.2	8.8	7.8 ± 0.4[b]	5.4	5.5	6.6	5	2.7	−1.5
GaAs	13.3	$10.7\sim11.7$	7.4	5.0	4.6	...	6.2	...	1.5	...
GaSb	16.1	14.7	10	7.5	6.5	6	8.5	5	3.1	...
GaP	8.6	10.5 ± 1.6	3.5	5.8	1.8	...	2.1	...	−1.7	−1.1
InAs	11.1	$9.6\sim10.8$	6.3	7.0	3.5	...	4.8	...	−0.02	...
InP	13.4	8.5	7.5	...	4.6	...	6.8	...	1.8	...
InSb	15.2	$15.5\sim17.6$	9.5	8.5	5.9	6	8.3	...	2.7	...
AlSb	14.7	10 ± 2	7.5	...	4.0	...	6.4	...	0.5	−1.5
ZnTe	8.1	7	4.0	6.0[c]	1.3	...	3.0	...	−1.6	...
ZnSe	5.8	7	2.5	...	−0.3	...	1.4	...	−3.7	−2
ZnS	3.6	6.5 ± 1	0.86	...	−1.9	...	−0.1	...	−5.2	...
CdTe	2.8	8	1.5	6.0[c]	−1.0	...	0.5	...	−4.3	...

[a] E_0 is taken as the transition $\Gamma_{15,v}\rightarrow\Gamma_{1,c}$ (or $\Gamma_{15,v}\rightarrow\Gamma_{15,c}$ for Si) (in zinc-blende notation), which is the top valence band state and lowest conduction one at the Brillouin zone center. E_1 is identified as the gap at $k=(2\pi/a)$ (0.5, 0.5, 0.5), E_X as the gap at $k=(2\pi/a)$ (1, 0, 0). The indirect gaps $E_{\Gamma L}$ and $E_{\Gamma L}$ are identified as the energies of the lowest conduction states at $k=(2\pi/a)$ (0.5, 0.5, 0.5) and $k=(2\pi/a)$ (1.0, 0.0, 0.0) [or $k=(2\pi/a)$ (0.85, 0.0, 0.0) for Si], respectively, measured from the top of the valence band at zone center. All the pressure coefficients are calculated assuming linear variations of band gaps between $p=1$ bar to 20 kbar.

[b] Reference 2.

[c] C. D. Langer, in *Proceedings of the Seventh International Conference on the Physics of Semiconductors, Paris*, 1964, edited by M. Hulin (Dunod, Paris, 1964), p. 241. All other experimental values are those cited in Ref. 9.

density; $E_g(\hbar\omega_g)$ is the average Penn gap[14]; and

$$f_H(\vec{q})=\frac{0.5}{1+K_s^2/q^2+K_F^2/q^2}\quad(\text{here } K_s=2K_F/\pi)$$

is the Hubbard exchange and correlation correction.[16] It should be pointed out that for values of $\vec{q}$ relevant to the present calculation, $\epsilon^*(\vec{q})$ agrees very well with the results obtained from more sophisticated calculations.

The pressure dependence of $\epsilon^*(\vec{q})$ can readily be calculated provided the pressure dependence of E_g is known. In the present work, we shall determine dE_g/dp self-consistently by requiring the value used in calculating the change of $\epsilon^*(\vec{q})$ with pressure to be equal to the pressure coefficient of the band gap at $\vec{k}=(2\pi/a)(0.5, 0.5, 0.0)$. This latter identification is suggested by various theoretical and experimental studies of the optical spectra of the crystals considered: In his original calculation[17] of the optical spectra of Si and Ge, Brust found that the strongest peak in the ϵ_2 spectrum (imaginary part of the dielectric constant) of these crystals was the result of two nearly degenerate critical-point transitions, $X_{4,v}\rightarrow X_{1,c}$ and $\Sigma_{2,v}\rightarrow\Sigma_{3,c}$. The former is located at $\vec{k}=(2\pi/a)(1, 0, 0)$, the latter at $\vec{k}\approx(2\pi/a)(0.5, 0.5, 0)$. Heine and Jones[18] later gave a heuristic interpretation of the optical spectrum of diamond-type crystals. They showed that the region of the Brillouin zone (BZ) which embraces the two transitions and their vicinities can, in fact, be mapped onto the surfaces of a Jones zone, which contains four times the volume of the BZ and is a good approximation to the Fermi "sphere" of these crystals. If one assumes that the energy bands within the Jones zone are approximately free-electron-like, except near the zone boundaries, where they have nearly constant energy gaps, then one would expect the optical spectrum to consist of a single strong oscillator with energy roughly equal to $E(X_{4,v}\rightarrow X_{1,c})$ or $E(\Sigma_{2,v}\rightarrow\Sigma_{3,c})$. This, however, is almost identical to the Penn model,[14] which has an isotropic free-electron energy band throughout, except near the Fermi surface, where it has a gap E_g, the Penn gap. The work of Heine and Jones is significant in that on the one hand, it lends physical insight into the conclusions reached by Brust via detailed calculations, while on the other hand, it justifies the simple Penn model as applied to tetrahedrally bonded semiconductors. More recent theoretical[19] and experimental[20] investigations have identified and/or confirmed similar origins of the strongest peak in the optical spectrum of most compound semiconductors. However, the contribution from the $\Sigma_{2,v}\rightarrow\Sigma_{3,c}$ transition is found to be far more predominant. In the present work, we find that better results are indeed obtained by identifying E_g as the gap at $\vec{k}\approx(2\pi/a)(0.5, 0.5, 0)$ rather than at $\vec{k}=(2\pi/a)(1, 0, 0)$. Similar identification of E_g was also made previously by Brust.[15]

III. PRESSURE DEPENDENCE OF BAND GAPS

In Table I, we present the pressure coefficients of several important band gaps, direct as well as

indirect, of Si, Ge, and the II-V and III-V semiconductors. The form factors of Cohen and Bergstresser[21] have been used. For all the semiconductors considered, the agreement of calculated coefficients with experiment is uniformly good for most of the gaps, with the possible exception of the indirect gap $E_{\Gamma X}$. The calculated pressure coefficients are generally within 25% or so of experimental values, which we feel is within experimental uncertainty. As for the discrepancy that exists between the calculated and experimental coefficients of $dE_{\Gamma X}/dp$, the following comment can be made: It is found the $dE_{\Gamma X}/dp$ is extremely sensitive to small changes in PFF's. Since all the calculated $dE_{\Gamma X}/dp$ are rather small in magnitude, it is felt that slight modification on the PFF's might effectively reverse the sign of calculated $dE_{\Gamma X}/dp$. This is manifested in the case of GaP, where a negative $dE_{\Gamma X}/dp$ is predicted, in agreement with experiment. Also in Si, we found that the indirect gap $E_{\Gamma X}$ first increases with p, then decreases, so that $E_{\Gamma X}$ at 10 kbar is larger than at 20 kbar; this shows nonlinearity of $E_{\Gamma X}$ as a function of pressure, which could be important, at least in Si.

Previous high-pressure band-structure calculations (except those by Melz) were concerned with elemental group-IV semiconductors such as Si and Ge. A comparison with these calculations reveals that except for the indirect gap $E_{\Gamma X}$, our calculated pressure coefficients for other important band gaps are at least in as good agreement with experimental data as those obtained from more complicated models. For III-V compounds, our results are definitely in better agreement with experiments than Melz's, which are the first high-pressure band-structure calculations for these crystals. Regarding the fact that in our calculations only the compressibility and normal-pressure PFF's are used as input data, the good agreement obtained, particularly for direct gaps, is rather gratifying. The fact that the pressure coefficients of direct gaps are accurately predicted in the present work would make our simple scheme useful for calculations of the pressure dependence of optical spectra, where usually only direct electronic transitions are taken into account.[10] It is also of interest to point out that the success of the present scheme seems to imply that the q dependence of the Fourier transform of the pseudopotential is well represented by the empirically determined PFF's, so that a numerical interpolation scheme as described here is adequate for determining the high-pressure PFF's. Furthermore, along with the "tranferability" of atomic (ionic) pseudopotentials,[10] the scheme can also be effectively used to calculate the band structure of hitherto unexplored crystals composed of atoms (ions) whose PFF's have been determined from other calculations.

The analogous calculations for II-VI compounds, however, yield results which are rather disappointing. For example, the calculated dE_0/dp are much too small compared with experimental data. This seems to stem from too strong a pressure dependence of the antisymmetric PFF's, especially the $V^A(3)$ component. Because of this, results in Table I are based on calculations in which the antisymmetric PFF's are assumed to be totally independent of pressure. Except for CdTe, the E_0-gap pressure coefficients are in fair agreement with available experimental data. Although no rigorous justification can be made for this procedure, a partial justification is forthcoming from the quantum dielectric theory of Phillips and Van Vechten,[22] where the hetropolar (ionic) energy gap C is some sort of average of the antisymmetric PFF's. Van Vechten[22] further arrives at the conclusion that for highly ionic crystals, $dC/dp \approx 0$. He argues that since the Madelung energy makes the dominant contribution to the cohesive energy in highly ionic crystals, the condition $dC/dp \approx 0$ is compatible with the condition that the equilibrium lattice constant maximizes C, and hence the cohesive energy of the crystals. This very condition was, in fact, employed by Camphausen *et al.*[9] in their calculation of the pressure coefficients of band gaps, which is based on a modified version of the quantum dielectric theory. Since II-VI semiconducting compounds are more ionic than III-V's, we expect their antisymmetric PFF's to be less pressure dependent. Hence, as a first approximation, they are assumed to be independent of pressure.

IV. PRESSURE DEPENDENCE OF REFRACTIVE INDEX

The recent emergence of a variety of high-power laser applications has generated much interest in the careful determination of parameters characterizing optical distortion phenomena in solids.[23] Included among the latter parameters is dn/dp, the pressure derivative of the refractive index, which characterizes pressure-induced distortion. The frequency regime of interest for optically transmitting materials is the transparent region well below the energy gap ω_g but well above the fundamental phonon resonance ω_0. We will here be concerned with dn/dp for pure semiconductors, where only band-to-band electronic contributions need be considered. Lattice contributions are negligible for all practical purposes, except very near to ω_0; likewise, free carrier effects are negligible in pure materials at reasonable temperatures, except for very narrow gap materials which will not be of interest here.

Camphausen *et al.*[9] (CCP) calculated dn/dp employing the modified version of Van Vechten's di-

TABLE II. dn/dp of semiconductors.

Crystal	$K(10^{-6}/\text{bar})$	$\omega_g(\text{eV})$[a]	ϵ_e	$\frac{d\omega_g}{dp}$ (10^{-6} eV/bar)	$\frac{1}{n}\frac{dn}{dp}$ (10^{-6}/bar) this work	CCP[b]	Experiment[c]
Si	1.02	4.8	12.0	4.1; 3.1,[d] 2.6[e]	−0.31	−0.3 ± 0.05	−0.3
Ge	1.33	4.3	16.0	7.0; 5.8,[d] 4.6[e]	−0.89	−1.0 ± 0.2	−0.7 to −1.0
GaSb	1.77	4.1	14.4	9.1	−1.23	−0.8 ± 0.2	...
GaAs	1.34	5.2	10.9	5.9	−0.44	−0.5 ± 0.2	−0.7 ± 0.1
InSb	2.20	3.7	15.7	9.2	−1.30	−1.1 ± 0.2	...
InAs	1.72	4.6	12.3	5.9	−0.39	−0.7 ± 0.2	...
GaP	1.13	5.8	9.1	2.0	+0.20	−0.3 ± 0.2	...
AlSb	1.69	4.7	10.2	5.7	−0.33	−0.5 ± 0.2	...
InP	1.38	5.2	9.6	6.2	−0.45	−0.4 ± 0.2	...
ZnS	1.39	7.8	5.2	1.9	+0.36	0.05 ± 0.1	−0.1
ZnTe	2.00	5.8	7.3	4.9	+0.14	0.01 ± 0.1	...
ZnSe	1.70	7.4	5.9	3.5	+0.32	0.07 ± 0.1	...
CdTe	2.36	5.5	7.2	3.8	+0.53	0.1 ± 0.1	...

[a]Reference. 22.
[b]Reference. 9.
[c]Values cited in Ref. 9.
[d]Calculated values in Ref. 4.
[e]Calculated values in Ref. 6.

electric theory, as mentioned above. Here we make use of results obtained in the last section to calculate dn/dp of diamond and zinc-blende-type semiconductors.

Adopting an approach similar to that employed by Tsay *et al.*[24] for calculating the temperature dependence of n, one takes for $\omega_g \gg \omega \gg \omega_0$, where ω_0 is the long-wavelength transverse-optic phonon frequency

$$\epsilon_e = n^2 = 1 + \omega_p^2/\omega_g^2 , \tag{6}$$

where ω_p is an effective plasma frequency and ω_g is an effective band gap, taken here simply as the gap at the point $k = 2\pi a^{-1}(\frac{1}{2}, \frac{1}{2}, 0)$ of the Brillouin zone as discussed above. From (6) one obtains

$$n^{-1}\frac{dn}{dp} = \tfrac{1}{2}(1 - \epsilon_e^{-1})\left(K - 2\omega_g^{-1}\frac{d\omega_g}{dp}\right) , \tag{7}$$

where K is the isothermal compressibility. The latter is known reasonably accurately for most crystals; thus, the central task becomes the evaluation of $d\omega_g/dp$. A similar approach was suggested by Heine and Jones,[18] although no detailed calculations were performed.

The final calculated values of $d\omega_g/dp$ and dn/dp are listed in Table II, alongside the calculated values of CCP and available experimental data.[25] Our values for dn/dp are observed to be similar to those of CCP for diamond and III-V crystals, except for GaP. The origin of the positive value of dn/dp for GaP is an unusually small value of $d\omega_g/dp$ calculated for this crystal. In the case of II-VI's, however, our results differ substantially from those of CCP. The present calculated values display good agreement with experiment for Si and Ge, fair agreement for GaAs, and poor agreement for ZnS. Some comments are in order regarding our results for the II-VI's: On the one hand, the trend to more positive values for the II-VI's is in agreement with the larger values of K and ω_g associated with increasingly ionic materials (dn/dp is large and positive for highly ionic materials such as alkali halides). However, it must be pointed out that since the agreement between our calculated pressure coefficients of band gaps and experimental data for II-VI compounds is not as good as the cases for group IV and III-V compounds, the dn/dp calculated for the former might be less reliable, although adequate experimental data are not available at present for a more thorough comparison of theory with experiment. Also, for the II-VI compounds, aside from the uncertainty which results from the assumption of pressure-independent antisymmetric PFF's, another uncertainty appears to be the stronger variation in dE_g/dp for different points in the BZ not accounted for by the simple assignment discussed above.

V. REMARKS AND CONCLUSIONS

In the present paper, we have shown that a simpler scheme, in which only the compressibility and atmospheric-pressure PFF's are required, is fairly adequate for describing the pressure-dependent band structures of a large number of semiconductors. However, since the $\vec{q}$ dependence of PFF's is determined from their empirical values by numerical interpolation, the results for each crystal calculated within the present scheme are necessarily dependent on the particular set of empirical PFF's used. We found that the Cohen-Bergstresser empirical PFF's on the average gave

better results compared with experimental data, even though rather similar results are obtained for a slightly different set of PFF's. We believe that the present scheme is sufficiently simple and accurate to be useful in calculating pressure-dependent band structures, and also optical spectra of semiconductors. Previously, the present authors demonstrated the usefulness of the empirical pseudopotential method for calculating the temperature derivative of the refractive index of semiconductors. The present results show that the same method is also a promising one when applied to the calculation of the pressure derivative of the refractive index.

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*Support by Air Force Cambridge Research Laboratories (AFSC) under Contract No. F19628-72-C-0286.

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