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Crystal Potential and Energy Bands of Semiconductors. II. Self-Consistent Calculations for Cubic Boron Nitride*

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A self-consistent crystal potential is constructed for cubic BN. Exchange is included according to the Slater free-electron approximation. The effect of the heteropolar character of the potential is included explicitly in an approximately self-consistent treatment of the valence-electron charge density. The energy gap is found to be about twice that of diamond, consistent with the results of other zincblende crystals and their diamond-type analogs. The maximum of valence band and the minimum in the conduction band are at the center and (100) face of the Brillouin zone, respectively. It is suggested that the heteropolar potential splits the valence band into two sub-bands. The lower sub-band width is about 5 ev, while the higher (which contain three times as many states) has a band width of about 4 ev. The energy gap between the sub-bands is about 10 ev. The effect should be common to all zincblende crystals and may be observable by soft x-ray emission.

1. INTRODUCTION

In recent years a great deal of experimental information has been obtained relating to the energy bands of III-V zincblende crystals.[1] This information suggested some time ago to Herman[2] that the heteropolar zincblende crystals can be regarded as perturbed homopolar diamond-type crystals. This perturbation consists primarily of two terms, one coming from the atomic cores and the other from the valence electrons. The first term, which is the larger, consists chiefly of the ionic potential derived from the difference of nuclear charges. This ionic potential perturbs the valence electron distribution so that more electrons are found near the group V ion than the group III ion: the valence electrons have screened the ionic potential and the "effective charge" is less than one.

An accurate calculation of a zincblende crystal potential requires the calculation of both terms. Dependable results can only be expected, however, if they are obtained for the diamond-type analog of the zincblende crystal. So far this has been accomplished only in Herman's calculations of the energy bands of diamond.[3] In the first paper[4] (I) of this series, we showed that Herman's diamond potential was approximately self-consistent. We shall now present self-consistent calculations for cubic boron nitride using the same methods; in so doing we take advantage of the fact that for atoms in the first row of the periodic table the core contribution to the crystal potential is known quite accurately. We are therefore focusing our attention on the screening effects produced by the valence electrons; it is our object to calculate these self-consistently. It should be the case that these effects will be quite similar in all zincblende crystals; using our methods it should be straightforward, e.g., to calculate the bands of AlP once the bands of Si have been calculated correctly.

In Sec. 2 we outline our general method for calculating the crystal potential. In Sec. 3 we present the results of the energy-band calculation. A critical comparison of the present approach with previous calculations based on the cellular approximation is given in the last section.

2. VALENCE CHARGE DENSITIES AND CRYSTAL POTENTIAL

The cubic form of BN has been prepared only recently.[5] The lattice constant is 3.615 A, which is about 2% larger than the lattice constant of diamond.

The calculations to be presented here were carried out using our "effective potential" formulation[6] of the OPW method; this formulation was also used in our study of diamond (I).[4] The boron 1*s* wave function was taken from the self-consistent calculations with exchange of Glembotski, Kibartas, and Iutsis.[7] These gave $E_{1s}{}^{B}=-15.4$ ry. The nitrogen 1*s* wave function was taken from the similar calculations of Hartree and Hartree.[8] They do not give the 1*s* energy but by comparing the result for boron and carbon ($E_{1s}{}^{C}=-22.7$ ry according to Jucys[9]) we estimate $E_{1s}{}^{N}=-31.4$ ry by extrapolating linearly the effective Z's of boron and carbon ($E_{1s}=Z_{\text{eff}}{}^2$). From the 1*s* wave functions we have calculated the Fourier coefficients of

$$[1s]=\left\{\int\psi_{1s}^*(r)d^3r\right\}\psi_{1s}(r),\tag{1}$$

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[6] J. C. Phillips and L. Kleinman, Phys. Rev. **116**, 287 (1959).

[7] Glembotski, Kibartas, and Iutsis, J. Exptl. Theoret. Phys. U.S.S.R. **29**, 617 (1955) [translation: Soviet Phys. JETP **2**, 476 (1956)].

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[9] A. Jucys, Proc. Roy. Soc. (London) **A173**, 59 (1939).

for boron and nitrogen. It was shown in reference 6 that while p states move in the crystal potential V_c, s states see an effective potential

$$V_e = V_c + V_r, \tag{2}$$

where

$$V_r = V_r^{\mathrm{B}} + V_r^{\mathrm{N}}, \tag{3}$$

$$V_r^{\mathrm{B}} = (E - E_{1s}^{\mathrm{B}})[1s]^{\mathrm{B}},$$
$$V_r^{\mathrm{N}} = (E - E_{1s}^{\mathrm{N}})[1s]^{\mathrm{N}}. \tag{4}$$

In order to compare the potential in BN with that of diamond it is convenient to split the potential into two parts,

$$V_e = V_e^s + V_e^a, \tag{5}$$

which are, respectively, symmetric and antisymmetric with respect to reflection about an origin located midway between the two atoms in the unit cell. With respect to the diamond lattice these potentials transform like Γ_1 and $\Gamma_{2'}$, respectively. (We use the notation for the irreducible representations of diamond of Herring[10] and of zincblende of Parmenter.[11]) Thus each can be expanded in a Fourier series,

$$V_e^s = \sum_\kappa V_\kappa^s \cos \boldsymbol{\kappa}\cdot\boldsymbol{\tau} \langle\kappa\rangle_{\Gamma_1},$$
$$V_e^a = \sum_\kappa V_\kappa^a i \sin \boldsymbol{\kappa}\cdot\boldsymbol{\tau} \langle\kappa\rangle_{\Gamma_{2'}}. \tag{6}$$

Here $\boldsymbol{\tau} = a8^{-1}(111)$ and $\langle\kappa\rangle_\alpha$ denotes a symmetrized combination of plane waves belonging to equivalent reciprocal lattice vectors and transforming according to the irreducible representation α.

If our crystal potential were a superposition of spherically symmetric atomic potentials $V^{\mathrm{B}}(r)$ and $V^{\mathrm{N}}(r)$ then

$$V_\kappa^s = V_\kappa^{\mathrm{N}} + V_\kappa^{\mathrm{B}}, \tag{7}$$

$$V_\kappa^a = V_\kappa^{\mathrm{N}} - V_\kappa^{\mathrm{B}}, \tag{8}$$

$$V_\kappa^{\mathrm{N}} = (1/\Omega_0)\int V^{\mathrm{N}}(r) \exp(i\boldsymbol{\kappa}\cdot\mathbf{r}) d^3r, \tag{9}$$

$$V_\kappa^{\mathrm{B}} = (1/\Omega_0)\int V^{\mathrm{B}}(r) \exp(i\boldsymbol{\kappa}\cdot\mathbf{r}) d^3r, \tag{10}$$

where $\Omega_0 = a^3/4$ is the volume of the unit cell. This is the case with respect to the core potential and using Eqs. (7) and (8) the valence contribution to the potential can also be represented in terms of valence contributions from B and N. The various contributions to V_κ^{N} and V_κ^{B} for the first few values of κ are listed in Table I together with the first few Fourier coefficients of $[1s]^{\mathrm{B}}$ and $[1s]^{\mathrm{N}}$. For simplicity we have used the value of V_{000} calculated by Herman for diamond (-2.87 ry); slight changes in this value do not affect the relative positions of the bands.

TABLE I. Fourier coefficients of the atomic potentials of boron and nitrogen. The core exchange potentials are taken to be the same as the one calculated for carbon by Herman.[a] The last column represents the sum of the second, third, fifth, and sixth columns. The V_{200}^{val} terms are significant only for the difference between the boron and nitrogen values.

$\frac{a}{2\pi}\cdot\boldsymbol{\kappa}$	$V_{\mathrm{coul}}^{\mathrm{core}}$	$V_{\mathrm{exch}}^{\mathrm{core}}$	$[1s]$	$V_{\mathrm{coul}}^{\mathrm{val}}$	$V_{\mathrm{exch}}^{\mathrm{val}}$	V_{crys}
			Boron			
(111)	0.383	0.020	0.0212	−0.111	0.051	0.343
(200)	0.292	0.019	0.0200	−0.030	0.014	0.295
(220)	0.150	0.017	0.0152			0.167
(311)	0.112	0.012	0.0128			0.124
			Nitrogen			
(111)	0.630	0.020	0.0099	−0.192	0.089	0.546
(200)	0.480	0.019	0.0095	−0.046	0.022	0.475
(220)	0.243	0.017	0.0087			0.260
(311)	0.181	0.012	0.0072			0.193

[a] See reference 3.

The method of calculation of the valence electron contributions to V_κ^s has already been discussed in I. The same methods were used here, with valence electron exchange determined by the Slater free-electron approximation. It will be observed that V_{eff}^s in BN is practically the same as in diamond. Furthermore $V^s \gg V^a$ so that V^a can be treated as a perturbation. For self-consistent calculations this approach has the advantage of rapid convergence. Now the unperturbed eigenfunctions of V^s are the same as in diamond. We split the valence electron charge density into two parts,

$$\rho = \rho^s + \rho^a, \tag{5$'$}$$

and each of these can be expanded in Fourier series,

$$\rho^s = \sum_\kappa \rho_\kappa^s \langle\kappa\rangle_{\Gamma_1},$$
$$\rho^a = \sum_\kappa \rho_\kappa^a \langle\kappa\rangle_{\Gamma_{2'}}. \tag{6$'$}$$

To first order in V^a, ρ^s is determined by V^s. In fact the effect of V^a on ρ^s turns out to be negligible. Thus ρ^s in BN is the same as in diamond. Hence the Coulomb and exchange contributions of ρ_s to V_s are the same as in diamond, and these have been calculated self-consistently in I. We have now to calculate ρ^a.

From the corresponding result for ρ^s we anticipate that ρ_κ^a will be appreciable only for the first one or two smallest values κ. In principle ρ_κ^a should be calculated by averaging $\rho_\kappa(\mathbf{k})$ over all occupied states of the valence band labeled by $\mathbf{k}$. As in I we shall replace this average by a sampling of wave functions at Γ, X, and L. We shall consider errors in this approximation later.

As an example of the perturbation calculation of ρ_κ^a consider the states at the top of the valence band at $\mathbf{k}=0$ which were labelled $\Gamma_{25'}$ in the diamond lattice. (In a tight-binding picture these levels consist of bonding p wave functions.) The perturbation V^a mixes this level with Γ_{15} (which may be labelled antibonding p) with the result that some charge is shifted from the boron half of the unit cell to the nitrogen half. Actually

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[10] C. Herring, J. Franklin Inst. **233**, 525 (1942).
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only the lowest Γ_{15} level (which is degenerate with $\Gamma_{25'}$ when $V=0$) mixes appreciably. If these two wave functions are expanded in Fourier series

$$\Gamma_{25'}=a_1(111)+a_2(200), \tag{11}$$

$$\Gamma_{15}=b_1(111)+b_2(220), \tag{12}$$

[where (IJK) is equal to $\langle(2\pi/a)(IJK)\rangle$ multiplied by a suitable normalizing factor] then

$$(\Gamma_{25'}|V^a|\Gamma_{15})=i[\sqrt{2}(a_2b_1+a_1b_2)(V_{111}{}^a+V_{311}{}^a)+(a_1b_1+2a_2b_2)V_{200}{}^a]. \tag{13}$$

The form factor $i\sin\boldsymbol{\kappa}\cdot\boldsymbol{\tau}$ has been included explicitly in (13), so that the values of $V_\kappa{}^a$ can be taken from Table I. Now (13) can be substituted in the 2×2 reduced secular equation between $|\Gamma_{25'}{}^{(1)})$ and $|\Gamma_{15}{}^{(1)})$ and new eigenvalues and eigenfunctions obtained. In this approach $|\Gamma_{25'}{}^{(1)})$ and $|\Gamma_{15}{}^{(1)})$ are regarded as quasi-degenerate and are treated by degenerate perturbation theory. Corrections due to mixing of, say, $|\Gamma_{25'}{}^{(1)})$ with $|\Gamma_{15}{}^{(2)})$ are very small and can be neglected.

The wave function obtained from this secular equation will have the form

$$|\Gamma_{25'}{}^{(1)})_{\mathrm{BN}}=(1+\epsilon^2)^{-1}\{|\Gamma_{25'})+i\epsilon|\Gamma_{15})\}, \tag{14}$$

and from (14) with the aid of Poisson's equation the nonzero Fourier coefficients of the Coulomb potential of this charge density can be calculated. It turns out that $\rho_\kappa{}^s$ is practically unchanged; terms of the form $(\Gamma_{25'}|\Gamma_{15})$ however transform like $\Gamma_{2'}$ and contribute to $\rho_\kappa{}^a$. The results for $V_\kappa{}^s$ and $V_\kappa{}^a$ for each of the wave functions included in the sampling of the valence band are listed in Table II. It was shown in I that in this sample terms from X and L should be weighted, respectively, 3 and 4 times as heavily as terms from Γ.

The Coulomb screening just calculated is reduced by exchange. In I we found that satisfactory results were obtained for diamond from the Slater free-electron approximation for exchange among the valence electrons. According to the Slater approximation valence electron exchange produces an effective potential proportional to $\rho^{\frac{1}{3}}$ where ρ is the valence electron charge density. In semiconductors ρ is nearly constant and can be written

$$\rho\sim1+\epsilon(111),\quad \rho^{\frac{1}{3}}\sim1+(\epsilon/3)(111). \tag{15}$$

Thus the (111) Fourier coefficient of the exchange potential can be obtained directly by a formal expansion of the charge density as in (15). We have checked our result against Herman's, which was obtained by numerical integration; the two are in good agreement. According to (15) the exchange screening is directly proportional to the Coulomb screening; thus the exchange potential associated with ρ^a is readily calculated. This completes the calculation of the crystal potential listed in Table I.

TABLE II. The contribution of charge densities representing different sub-Zones in the valence band to the Fourier coefficients of the crystal potential. The next to the last line lists the total $=\{\Gamma\}+\{X\}+\{L\}$. Each of the latter represents the contribution of each term multiplied by the degeneracy and weighting factors listed in columns 2 and 3. Column 4 gives the result for $V^a=0$ and columns 5, 6, and 7 the self-consistent results including V^a.

Term	Degeneracy	Weight	$V_{111}{}^s(0)$	$V_{111}{}^s$	$V_{111}{}^a$	$V_{200}{}^a$
Γ_1	1		0.0072	0.0074	0.0030	0.0018
$\Gamma_{25'}$	3		0.0146	0.0137	0.0077	0.0038
$\{\Gamma\}$		1	0.0510	0.0485	0.0261	0.0132
X_1	2		0.0101	0.0099	0.0014	0.0000
X_4	2		0.0097	0.0096	0.0018	0.0000
$\{X\}$		3	0.1188	0.1170	0.0192	0.0000
L_1	1		0.0035	0.0035	0.0000	0.0000
$L_{2'}$	1		0.0104	0.0104	0.0014	−0.0008
$L_{3'}$	2		0.0106	0.0104	0.0039	0.0005
$\{L\}$		4	0.1404	0.1388	0.0369	0.0008
Total			0.310	0.304	0.082	0.014
$\{\Gamma\}$ alone			0.408	0.387	0.209	0.105

TABLE III. Energies in ry of various terms in diamond and cubic BN, using the Slater free-electron exchange potential.

Diamond	Energy	Boron nitride	Energy
$\Gamma_1{}^{(1)}$	−2.41	$\Gamma_1{}^{(1)}$	−2.48
$\Gamma_{2'}{}^{(1)}$	0.35	$\Gamma_1{}^{(2)}$	0.31
$\Gamma_{25'}{}^{(1)}$	−0.80	$\Gamma_{15}{}^{(1)}$	−1.16
$\Gamma_{15}{}^{(1)}$	−0.35	$\Gamma_{15}{}^{(2)}$	−0.11
		$X_1{}^{(1)}$	−2.07
$X_1{}^{(1)}$	−1.64	$X_3{}^{(1)}$	−1.21
$X_4{}^{(1)}$	−1.29	$X_5{}^{(1)}$	−1.37
$X_1{}^{(2)}$	−0.28	$X_1{}^{(2)}$	−0.39
		$X_3{}^{(2)}$	−0.29
$L_1{}^{(1)}$	−1.55	$L_1{}^{(1)}$	−1.42
$L_{2'}{}^{(1)}$	−1.97	$L_1{}^{(2)}$	−2.16
$L_{3'}{}^{(1)}$	−1.14	$L_3{}^{(1)}$	−1.26
$L_1{}^{(2)}$	−0.14	$L_1{}^{(3)}$	−0.20
L_3	−0.14	$L_3{}^{(2)}$	−0.13
		$W_1{}^{(1)}$	−2.02
		$W_3{}^{(1)}$	−1.34
$W_1{}^{(1)}$	−1.60	$W_2{}^{(1)}$	−1.24
$W_2{}^{(1)}$	−1.28	$W_4{}^{(1)}$	−1.33
$W_2{}^{(2)}$	0.22	$W_1{}^{(2)}$	0.38
$W_1{}^{(2)}$	0.71	$W_3{}^{(2)}$	0.80
		$W_2{}^{(2)}$	0.04
		$W_4{}^{(2)}$	0.20
Eg	0.40	Eg	0.77

We must now consider the accuracy of our method of calculating the valence contributions to ρ^s and ρ^a. In I we argued that the value of ρ^s should be correct to within about 10%. This is essentially a consequence of the fact that $\rho^s(\mathbf{k})$ varies only slightly on going from Γ to X or L, as can be seen from Table II. The same result is valid for ρ^s in BN. It appears, however, that ρ^a varies substantially throughout the Zone. Let us define the energy difference between the highest "bonding" state in the valence band and the lowest "antibonding" state with which V^a mixes the former appreciably as $\Delta E(\mathbf{k})$. Then we see that this variation is caused by large changes in $\Delta E(\mathbf{k})$ throughout the reduced Zone. The values of $\Delta E(\mathbf{k})$ at Γ, L, and X, respectively, are 0.45, 1.0, and 2.6 ry. Thus the largest contribution to ρ^a comes from the neighborhood of Γ while the neighborhood of X makes a small contribution.

The question now arises as to the accuracy of our point sampling of what should be an integral. In this case we estimate that our values of $\rho_\kappa{}^a$ are correct to about 30%. This corresponds to a change in $V_\kappa{}^a$ which is quite small ($\lesssim 0.02$ ry) so that the energy bands that we calculate should not be sensitive to errors from this source. Although the values of $\rho_\kappa{}^a$ are of some intrinsic interest, the nonanalytic behavior of the energy surfaces near Γ makes more detailed calculations unattractive.

The value of $V_{200}{}^a$ listed in Table II suggests that the (200) x-ray diffraction spot should have an integrated intensity about 20 times smaller than the (111) spot. According to Wentorf[12] the observed ratio is high, and is consistent with this estimate; the data presently available do not allow a more quantitative comparison.

The values of $\rho_{111}{}^s$ and $\rho_{111}{}^a$ can be used if desired to calculate "effective" charges. Whatever the definition of effective charge the result will not have great utility. The maxima of the valence radial charge densities of neutral boron and nitrogen fall at about half the interatomic spacing in the crystal so that if free-atom wave functions are used in defining the effective charge these wave functions will overlap so extensively as to render the result meaningless.

It is possible to ask what point charges would give the same antisymmetric potential. This leads to a valence "screening" charge of about 0.3 for either $V_{111}{}^s$ or $V_{111}{}^a$; the "effective charge" is then about 0.7.

3. ENERGY BANDS

With the potential listed in Table II it is a straightforward matter to calculate the energy bands of cubic BN from those of diamond by using the perturbation methods described in the last section. The results are listed in Table III where they are compared with the corresponding levels in diamond. The energy bands are also shown in Figs. 1 and 2 for diamond and BN, respectively.

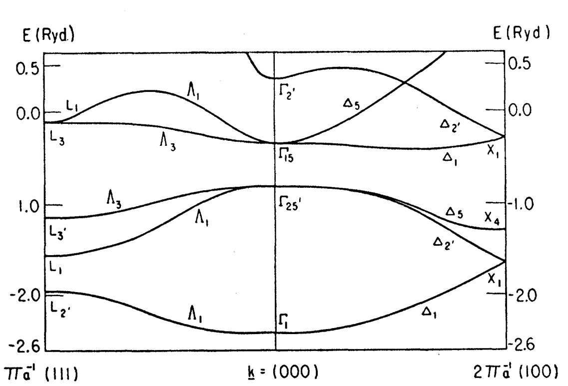

FIG. 1. A sketch of the energy bands of diamond along (100) and (111) axes of the Brillouin zone.

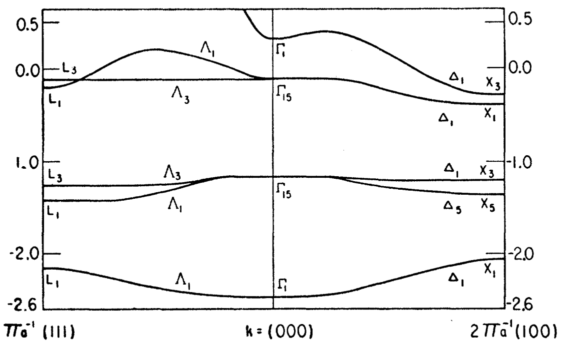

FIG. 2. A sketch of the energy bands of cubic BN. Note that the valence band is split into two sub-bands.

By comparison with the results previously obtained[13] for the energy bands of diamond-type lattices along Δ it seems highly probable that the minimum in the conduction lies at X. The energy gap is then about 10 ev, or about twice as large as the gap in diamond. It is interesting to note that the increase in the gap results from the depression of the top of the valence band, $\Gamma_{25'}$, by V^a through interaction with Γ_{15}. This is much larger than the depression of the conduction band through the splitting of the twofold degenerate level $X_1{}^{(2)}$. The latter splitting is quite small although in general it need not be (e.g., $X_1{}^{(1)}$ is split by a large amount). This results from a cancellation of terms involving $V_{111}{}^a$ and $V_{200}{}^a$. It is probable that the same mechanism is operative in AlP and accounts for the increase in energy gap of that crystal compared with Si (3.0 ev compared to 1.1 ev).

We have also calculated energy levels at W to check a suggestion by Callaway[14] based on group-theoretical considerations that the maximum in the valence band might shift to W in zincblende crystals. The valence band levels at W in diamond are twofold degenerate with W_2 lying nearer the top of the valence band. The splitting of W_2 is approximately proportional to $V_{111}{}^a - V_{200}{}^a$ while that of W_1 is proportional to $V_{111}{}^a + V_{200}{}^a$. Thus the splitting of W_2 is about 10 times smaller than that of W_1; this is readily understood in terms of the p and s characters, respectively, of the levels. None of the levels at W are found to be near $\Gamma_{25'}$, so that it appears quite likely that the maximum in the valence band will be very near Γ. This conclusion is reinforced by the consideration that throughout the Zone the levels near the top of the valence band have primarily p character, and for the reasons just discussed the shifts in these levels due to V^a may be expected to be small.

This argument may also be applied to the s-like valence bands. As we have just seen, V^a produces a large splitting of W_1; inspection of Table III shows that large splittings are also found at X and L. Similar behavior should occur at all points on the Zone surface.

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[14] J. Callaway, J. Electronics **2**, 330 (1957).

Thus it appears that V^a produces a large splitting of the valence band, with the upper sub-band containing three times as many states. The energy gap between sub-bands should be of the order of 6 ev in BN; in GaAs the sub-bands should be split by about 3 ev. This splitting should be observable in soft x-ray emission[15] or double Auger emission.[16]

The valence band width is reduced, compared to diamond, from 21.5 ev to 18.0 ev. This small narrowing is also consistent with the idea that BN is still predominantly homopolar.

4. COMPARISON WITH PREVIOUS WORK

Calculations for heteropolar semiconductors have been carried out previously by Bell *et al.*[17] for PbS and by Birman[18] for ZnS. Both calculations are subject to the criticism that they neglect exchange (an unavoidable approximation, since Hartree-Fock calculations are not available for Pb and Zn). From Herman's work[19] on Ge, however, it is known that omission of exchange can lead to the wrong order of *s* and *p* levels in the conduction band. Our chief concern here, however, is the treatment of the potential outside the core region. To study this point we compare our calculation with Birman's treatment of zincblende.

Birman uses the cellular approximation in which spheres are drawn around each atom; the potential is assumed spherically symmetric within the spheres and is zero outside the spheres. Application of the ordinary cellular method to a tetrahedrally coordinated lattice, where the largest radius of the atomic cell is twice the smallest radius is itself open to grave doubt; again this point is not our major concern. We wish to emphasize that the spheres constructed have no fundamental significance; the same remark applies to the "effective charge" contained within the spheres. The significant quantities are the Fourier coefficients of the crystal potential as defined in Eqs. (6)–(10) of Sec. 2 and as listed for BN in Table I.

The most important feature of the present approach is the ease and directness with which it leads to a *self-consistent* crystal potential. It is possible to obtain similar results using refined cellular methods (such as augmented plane waves) but if the potential varies appreciably outside the cores (which it does in diamond-type lattices) it would appear that achieving self-consistency would require rather more cumbersome calculations.

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