PHYSICAL REVIEW B VOLUME 32, NUMBER 12 15 DECEMBER 1985

Linearized augmented-plane-wave calculation of the electronic structure and total energy of tungsten

Su-Huai Wei and Henry Krakauer
Department of Physics, College of William and Mary, Williamsburg, Virginia 23185

M. Weinert
Department of Physics, Brookhaven National Laboratory, Upton, New York 11973
(Received 13 June 1985)

Local-density-functional calculations of the energy bands, equilibrium lattice constant, bulk modulus, and cohesive energy have been performed using a newly developed self-consistent full-potential linearized augmented-plane-wave (LAPW) program. Scalar-relativistic effects are included for the band states, and the core-level states are treated fully relativistically in a central-field approximation. Excellent agreement is obtained with the experimental lattice constant and bulk modulus. Generally good agreement is obtained with the scalar-relativistic pseudopotential results of Bylander and Kleinman. In this context, the impact of various approximations used in including the core states is assessed, and these findings are related to the frozen-core and pseudopotential approximations, especially with regard to the treatment of the somewhat overlapping $5p$ semicore states and their effect on ground-state properties. Comparison with the recent LAPW results of Jansen and Freeman yields remarkably consistent values of the total energy at the equilibrium volume and provides a strong check on the accuracy of these two independently developed bulk LAPW programs.

I. INTRODUCTION

There have been major advances in the last few years in *ab initio* theoretical methods for determining the electronic, vibrational (phonon), and crystallographic structure of solids, surfaces, and molecules using local-(spin)-density-functional L(S)DF theory.[1–13] Self-consistent L(S)DF calculations have yielded results for the total energy, pressure, and forces[10] acting on the nuclei as a function of crystal structure and volume. These calculations have provided information about not only the normal (ambient-pressure) properties, but also about the high-pressure equation-of-state and solid-solid phase transitions, and such calculations have become increasingly important in view of the growing number of high-pressure studies using diamond-anvil techniques.[14]

In this paper we report local-density-functional (LDF) calculations of the energy bands, equilibrium lattice constant, bulk modulus, and cohesive energy of tungsten, performed using a newly developed all-electron self-consistent full-potential linearized augmented-plane-wave (LAPW) code. Excellent agreement is obtained with the experimental lattice constant and bulk modulus, and good agreement is obtained with the experimental cohesive energy.

The LAPW results reported here are found to be in generally good agreement with the scalar-relativistic pseudopotential calculations of Bylander and Kleinman[15] (BK), the nonrelativistic pseudopotential calculation of Zunger and Cohen[16] (ZC), and a calculation using an independently developed LAPW program by Jansen and Freeman[17] (JF). Comparison with the results of JF provides a useful calibration of these two independently developed LAPW programs.

The underlying approximation of the pseudopotential approach is the frozen-core approximation, and, in this context, the effect of the overlapping tungsten $5p$ semicore states on the equilibrium properties is assessed in some detail. It is found that, at least near the equilibrium (zero-pressure) volume, these $5p$ "fat" core states have negligible effect on the predicted equilibrium volume and a small effect on the predicted bulk modulus.

In the next section the LAPW method is briefly reviewed. In Sec. III we present a discussion of the results obtained, and the primary conclusions are summarized in Sec. IV.

II. CALCULATIONAL METHOD

The calculations reported here were performed with a newly developed LAPW computer code for bulk crystals. The main features of this code compared to the earlier slab-LAPW code[18] are as follows. (1) No symmetry assumptions are used (e.g., such as the existence of a site of inversion). This is an important feature for total-energy and frozen-phonon calculations, since various distortions of an otherwise high-symmetry crystal may be required. (2) Like the earlier version, the representation of the potential charge and spin density are unrestricted by shape approximations (such as spherical muffin-tin potentials). (3) It is an all-electron method in that both core and valence states are treated self-consistently.

The LAPW method for obtaining the band eigenstates from augmented-plane-wave variational basis functions has been fully described in Refs. 18–20, and is summarized briefly here. For a periodic bulk crystal, all space is partitioned into two types of regions: (1) nonoverlapping muffin-tin spheres centered on each atom, and (2) the

remaining interstitial space between these spheres. A LAPW basis function consists of a plane wave in the interstitial region joined continuously and differentiably onto scalar-relativistic[21] solutions of the spherical component of the potential inside the muffin-tin spheres. The innermost core-level eigenstates are not usually treated variationally (except where stated otherwise), but are obtained using a fully relativistic atomiclike program using the spherical component of the muffin-tin potential. The core eigenstates are recomputed in each iteration, permitting the core states and core charge density to be determined self-consistently, as are the band eigenstates (i.e., no frozen-core approximation is made).

Although only the spherical component of the muffin-tin potential is used to construct the basis functions, the full potential including nonspherical components is treated in the variational determination of the band eigenstates. Thus, no "shape" approximations are employed for either the potential or the charge density.

The relativistic exchange potential[22,23] of MacDonald and Vosko[23] was used together with the Wigner[24] interpolation formula for the correlation potential. Relativistic corrections are included only for the exchange potential, since these corrections are most important in regions of high charge density, where exchange effects dominate correlation contributions.

The total energy is calculated within the LDF formalism using a method developed by Weinert *et al.*[11] This method is well suited to the LAPW method and is very stable numerically. This is important in all-electron total-energy calculations, since differences between total energies are much smaller than the total energy itself.

A well-converged basis set of about 80 LAPW's is used, resulting in differences between total energies which are converged to better than 0.1 mRy. The convergence of individual band eigenvalues is shown in Table I. The number of basis functions and the muffin-tin radii used for different lattice parameters was kept fixed. Inside the muffin-tin spheres, the LAPW's are expanded up to $l=8$, and the maximum l value used to construct the lattice harmonics is also $l=8$.[19,25,26] The rms error in the continuity of the charge density and potential is less than 0.2% in all cases.

The Brillouin-zone summations for the charge density are performed using a discrete k-point summation in which each eigenvalue is effectively broadened using an artificial Fermi-Dirac distribution corresponding to $kT=2$ mRy. This results in rapid convergence of these summations with respect to the number of k points used. In the initial self-consistent iterations, eight special[27] k points in the irreducible Brillouin zone are used to get close to self-consistency. The final iterations are carried out using a uniform mesh of 55 k points, and the change due to increasing the number of k points results is less than 2% in the bulk modulus and about 0.1% in the predicted lattice parameter.

Iterations are continued until the total energy is stable to 10^{-5} Ry. At this level of self-consistency the integrated rms difference between the input and the output charge density is of the order of 10^{-4} electrons bohr^{-3}.

III. RESULTS AND DISCUSSION

A. Equilibrium properties

The lattice constant and bulk modulus of tungsten are obtained from the calculated total energies as a function of volume in the bcc crystal structure. Total energies are calculated at four different lattice parameters ranging from 3% smaller to 3% larger than the experimental[28] lattice constant. The results are shown in Table II. The calculated total energies are then fitted to Murnaghan's equation of state[29]

$$E(V)=\frac{B_0 V}{B_0'}\left[\frac{(V_0/V)^{B_0'}}{B_0'-1}+1\right]+\text{const}\,, \tag{1}$$

where B and B' are the bulk modulus and its pressure derivative at the equilibrium volume V_0. In Table III the lattice constant, bulk modulus, and cohesive energy obtained from this fit are compared with those calculated by BK,[15] ZC,[16] and JF,[17] as well as with experiment.[30–34] BK, ZC, and JF fitted their total-energy results to a polynomial in the lattice parameter, and we have also tested some other functional forms for the equation of state. We found that in tungsten the lattice parameter is rather insensitive to the particular form used, over this range of volumes. Assuming a quadratic expansion in the lattice parameter, the equilibrium lattice parameter changes by only 0.3% compared to the value obtained from Murnaghan's equation. The bulk modulus changes by only 1.5%. The calculated pressure derivative B' obtained from Murnaghan's equation is 4.88, in good agreement with the experimental value of 4.32.[30]

To obtain the cohesive energy of bulk tungsten, self-consistent spin-polarized[5] all-electron atomic calculations were performed for the isolated tungsten atom using the von Barth—Hedin[2] spin-density functional. As the nonspin-polarized limit of the von Barth—Hedin functional is the Hedin-Lundqvist[35] density functional, we repeated the bulk calculation using the Hedin-Lundqvist density functional. Since in the bulk calculation the $5d$ and $6s$ states

TABLE I. Convergence of selected band states with number of augmented plane waves. PW1 and PW2 are the number of plane waves in two calculations, and ΔE is the difference between the eigenvalues of these two calculations (in meV).

	Γ_{15}	$\Gamma_{25'}$	P_4	N_1	N_2	$N_{1'}$
PW1	55	55	68	68	68	68
PW2	79	79	80	80	80	80
ΔE	0.02	21.4	1.70	0.79	4.02	0.84

TABLE II. Calculated total energy (Ry) at four lattice parameters (Å).

a	E
3.064	−32 244.305 59
3.160	−32 244.316 78
3.207	−32 244.314 87
3.256	−32 244.308 95

are treated scalar relativistically while the other states are treated fully relativistically, this was also done in the atomic calculation. The bulk equilibrium total energy is −32 313.017 Ry, and the isolated-atom total energy is −32 312.275 Ry. The cohesive energy is thus 10.09 eV. The corresponding values in the calculation of JF (Ref. 17) (who used the Hedin-Lundqvist exchange-correlation potential throughout) are −32 313.018 for the bulk, −32 312.300 for the spin-polarized atom, and a cohesive energy of 9.76 eV. This constitutes truly remarkable consistency between two independently developed LAPW programs. We are not certain of the cause of the somewhat larger discrepancy in the two atomic calculations. The discrepancy with experiment is about 1.0—1.2 eV in these calculations. We attribute this overestimate of the cohesive energy E_c to neglected multiplet effects in the atom, which would tend to increase the binding energy of the atom and thus reduce the calculated cohesive energy. In view of this, the near-perfect agreement in Table III between BK's E_c and experiment is hard to understand. The low E_c for ZC may be due to the neglect of scalar-relativistic effects.

These results are summarized in Table III. The overall agreement with experiment[28,30–34] is very good.

B. Overlapping core-state effects

As mentioned, the core-electron states were treated self-consistently in an atomiclike approximation in obtaining the results given in Tables I—III. The handling of the core electrons in tungsten deserves some attention, since the $5p$ level is a "fat" core state (i.e., the $5p$ core state has about 0.1 electrons per unit cell outside of the muffin-tin spheres). This means, of course, that there is some overlap of $5p$ core states from neighboring atoms. This raises the question of how much these states contribute to the observed equilibrium properties. In addition, the effect of these "fat" core states can be expected to become more significant in high-pressure studies.

We now assess the impact of various approximations to the core states, and we relate our findings to the commonly used frozen-core and pseudopotential approximations. Tables IV and V display our results for various treatments of the core electrons. For each treatment, self-consistent calculations were carried out for the total energy at only three lattice constants, $a/a_0=0.97$, 1.0, and 1.03, where $a_0=3.160$ Å is close to the experimental value. The total energies are then fitted to a quadratic equation to obtain the equilibrium lattice constant and bulk modulus.

In calculation (1) in Tables IV and V the crystal core charge is treated self-consistently (the so-called soft-core approximation) in an atomiclike approximation. The atomiclike core-electron states for each atom are obtained in each iteration from the spherical part of the potential in each muffin-tin sphere extrapolated to infinity. The extrapolation procedure (a $1/r$ form was used) is somewhat arbitrary and calls into question the validity of this approximation. In bulk tungsten near the equilibrium volume, however, we have found that the results are insensitive to the specific form used. The crystal core charge density is then defined as the superposition of these spherical core charge densities. This crystal core charge density is then decomposed into a lattice harmonic expansion within the spheres (it contains nonspherical contributions coming from neighboring atoms) and a plane-wave expansion in the interstitial region.

In calculation (2) in Tables IV and V the atomiclike core states are obtained for each atom as in calculation (1). Instead of superposing these core densities, however, any "spill-out" core charge from the muffin-tin sphere is uniformly distributed in the interstitial region. The total spill-out core-state charge is 0.11 electrons, of which

TABLE III. Comparison of calculated lattice constant, bulk modulus and its pressure derivative, and cohesive energy E_c with experiment. The lattice parameter is in Å and the bulk modulus is in Mbar.

	ZC	BK	JF	LAPW	Expt.
a	3.173	3.162	3.149	3.164	3.162
B	3.45	2.97	3.45	3.18	3.1415[a] 3.1078[b] 3.232[c] 3.07[d]
B'				4.1	4.32[d]
E_c	7.90	8.93	9.76	10.09	8.90[e]

[a]Reference 33, $T=0$ K, extrapolated.
[b]Reference 33, T is room temperature.
[c]Reference 31.
[d]Reference 30, T is room temperature.
[e]Reference 34.

TABLE IV. Comparison of various treatments of the core-electron states (see text). The lattice parameter is in Å and the bulk modulus is in Mbar.

Core treatment	a	B
(1) Self-consistent, overlapping, atomiclike	3.168	3.24
(2) Self-consistent, atomiclike, constant Q_I	3.170	3.30
(3) Same as (2) but frozen core	3.164	3.78
(4) Same as (2) but renormalized frozen core	3.221	3.94
(5) Variational $5p$ core state, frozen inner core	3.171	3.66
(6) Same as (5) but self-consistent inner core	3.166	3.41
(7) Same as (1) but no spin-orbit for $5p$ core state	3.165	3.47
(8) Same as (1) but no spin-orbit for all core states	3.167	3.46
Experiment	3.162	3.142[a] 3.232[b]

[a]Reference 33.
[b]Reference 31.

about 90% comes from the $5p$ orbitals. As seen in Table V, the difference between the total energy in calculations (1) and (2) is rather small. The largest difference occurs at the smallest lattice parameter, where the atoms are closer together and core overlap is greater. We conclude that, at least near the equilibrium volume, the constant interstitial core charge density effectively simulates the overlap of the fat $5p$ core state.

The effect of the frozen-core approximation is examined in calculations (3) and (4) in Tables IV and V. The core charge density obtained in calculation (2) is used for this purpose. This approximation (3) leads to about a 20% error in the calculated bulk modulus. Calculation (4) further examines the sensitivity to the choice of the frozen-core charge density. The same initial frozen core is used as in (3), except that this core charge density is renormalized such that the number of core electrons inside the muffin-tin sphere is exactly 68, and there are *no* core electrons in the interstitial region. This core density is then frozen and used at all three lattice parameters. This results in even larger discrepancies in not only the bulk modulus but also in the predicted equilibrium lattice parameter. Calculations (3) and (4) thus show the magnitude of soft-core effects that can be expected in systems with fat core states.

We now examine the adequacy of treating the $5p$ fat core state as an atomiclike state. Calculations (5) and (6) in Tables IV and V treat the $5p$ level as a variational band state. In (5) the innermost core states were renormalized and frozen as in calculation (4). In calculation (6) the innermost core states were not renormalized or frozen, but were calculated self-consistently as in (1). The LAPW variational calculation was performed in two energy "windows," one for the conventional $5d,6s$ band states and one for the lower-lying $5p$ states. Thus, two different sets of LAPW energy parameters are used. This requires two separate diagonalizations of the secular equations at each k point, but yields the greatest variational freedom. Although this procedure correctly treats the $5p$ overlap, it neglects the spin-orbit splitting of the $5p$ levels (which is large, about 6.0 eV), since the band states are calculated scalar relativistically. [Spin-orbit effects are further examined in calculations (7) and (8).] Thus, the difference in total energy between (1) and (6), about 0.3 Ry, is due to the neglect of the $5p$ spin-orbit interaction. As expected, freezing the innermost core states which are very localized has very little effect. There is roughly a 12% error in the predicted bulk modulus in calculations (5) and (6), but these results are in better agreement with calculations (1), (2), and experiment than are the frozen-core calculations.

Finally, we examine spin-orbit effects. In the future we will implement the treatment of the spin-orbit interaction for the variational band states. For now, however, it is very easy to remove the spin-orbit interaction from the calculation of the atomiclike core states. This is done in calculations (7) and (8) in Tables IV and V. The only difference between calculations (1) and (7) is that the spin-orbit interaction has been removed from the $5p$ atomiclike core state. The results for the bulk modulus and the equilibrium lattice parameter are in very good agreement with calculation (6). Calculation (8) shows the effect of removing the spin-orbit interaction from all the core states. As expected, this further change has little effect on the equilibrium properties, since the remaining core states are extremely localized.

We conclude from these calculations that $5p$-core-state overlap has a significant impact on the elastic properties of tungsten, even at normal pressure, and that these effects can be expected to get larger at the reduced volumes obtained in high-pressure studies. The inclusion of the spin-orbit interaction of the $5p$ core state also has a significant effect on the bulk modulus, and this should also become increasingly more important at high pressure. These results also indicate that, at least for normal pressure, it is not necessary to treat the fat core states as band states. The frozen-core approximation, however, introduces significant errors. We believe this accounts for the better agreement of our calculated bulk modulus with experiment than had been previously obtained in the pseudopotential calculations of BK (Ref. 15) and ZC (Ref. 16).

C. Band structure

The calculated band structure along symmetry lines is displayed in Fig. 1. Table VI compares selected LAPW eigenstates with the scalar-relativistic pseudopotential eigenstates of BK and with the nonrelativistic results of

TABLE V. Total energy (Ry) at the three lattice parameters used in Table IV, $a/a_0=0.97$, 1.0, and 1.03, where $a_0=3.160$ Å ($-32\,244$ Ry has been subtracted from all the total energies).

Core treatment	a/a_0 0.97	1.0	1.03
(1) Self-consistent, overlapping, atomiclike	−0.305 59	−0.316 78	−0.308 95
(2) Self-consistent, atomiclike, constant Q_I	−0.305 03	−0.316 77	−0.309 09
(3) Same as (2) but frozen core	−0.304 82	−0.316 77	−0.306 55
(4) Same as (2) but renormalized frozen core	−0.263 77	−0.290 77	−0.294 11
(5) Variational $5p$ core state, frozen inner core	−0.003 37	−0.016 63	−0.008 35
(6) Same as (5) but self-consistent inner core	−0.007 02	−0.018 24	−0.009 44
(7) Same as (1) but no spin-orbit for $5p$ core states	−0.003 32	−0.014 60	−0.005 49
(8) Same as (1) but no spin-orbit for all the core states	46.381 91	46.393 40	46.384 61

ZC. Generally good agreement is obtained with the band structure of BK. Below the Fermi energy, the eigenvalues differ by about 0.1—0.2 eV. The agreement with the nonrelativistic results of ZC is considerably worse. The most notable case here is the much smaller $\Gamma_{25'}$-Γ_1 gap in ZC's results. This 3.55-eV discrepancy is a scalar-relativistic effect, which lowers predominantly s states relative to d states.

TABLE VI. Comparison of eigenvalues (in eV) at symmetry points in the Brillouin zone. All eigenvalues have been shifted so that the $\Gamma_{25'}$ eigenvalues are the same.

	ZC	BK	LAPW
Γ_1	3.551	0.165	0.000
$\Gamma_{25'}$	8.351	8.351	8.351
Γ_{12}	11.861	11.776	11.825
N_1	4.111	3.417	3.295
N_2	6.020	6.036	5.994
$N_{1'}$	11.441	10.662	10.448
N_1	11.761	11.684	11.707
N_4	12.471	12.600	12.710
N_3	14.581	15.504	15.894
H_{12}	3.731	3.794	3.695
$H_{25'}$	13.991	14.557	14.852
P_4	6.871	6.710	6.670
P_3	12.551	12.754	12.870

IV. CONCLUSIONS

We have reported local-density-functional calculations of the energy bands, equilibrium volume, bulk modulus, and cohesive energy of tungsten using a newly developed self-consistent full-potential LAPW code. Excellent agreement is obtained with the experimental lattice constant and bulk modulus, and good agreement is obtained

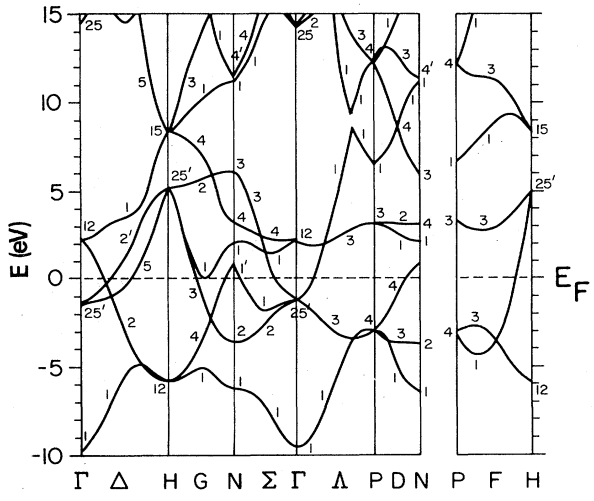

FIG. 1. Energy bands of scalar-relativistic tungsten with lattice constant $a_0=5.972$ a.u.

with the experimental cohesive energy. Generally, good agreement was also found with the scalar-relativistic pseudopotential calculations of Bylander and Kleinman,[15] the nonrelativistic pseudopotential calculation of Zunger and Cohen,[16] and a calculation using an independently developed LAPW program by Jansen and Freeman.[17] Comparison with the results of JF yielded remarkably consistent values of the total energy at the equilibrium volume and provides a strong check on the accuracy of these two independently developed bulk LAPW programs. The effect of the fat tungsten $5p$ core state on the equilibrium properties was also investigated in detail. It is found that, at least near the equilibrium (zero-pressure) volume, these $5p$ fat core states have negligible effect on the predicted equilibrium volume and a small effect on the predicted bulk modulus.

ACKNOWLEDGMENTS

One of us (H.K.) gratefully acknowledges many stimulating discussions with Warren E. Pickett during the course of developing this program. During this period, two of us (S.W. and H.K.) benefited from comparisons with unpublished band-structure calculations of tungsten which were kindly sent by Dale Koelling. This research was supported by the National Science Foundation under Grant No. DMR-81-20550.

[1]P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964); W. Kohn and L. J. Sham, *ibid.* **140**, A1133 (1965).
[2]U. von Barth and L. Hedin, J. Phys. C **5**, 1629 (1972).
[3]O. Gunnarsson, B. I. Lundqvist, and S. Lundqvist, Solid State Commun. **11**, 149 (1972).
[4]A. K. Rajagopal and J. Callaway, Phys. Rev. B **7**, 1912 (1973).
[5]V. L. Moruzzi, J. F. Janak, and A. R. Williams, *Calculated Electronic Properties of Metals* (Pergamon, New York, 1978).
[6]S. Froyen and Marvin L. Cohen, Phys. Rev. B **29**, 3770 (1984).
[7]K. Kunc and Richard M. Martin, Phys. Rev. Lett. **48**, 406 (1982).
[8]M. T. Yin and Marvin L. Cohen, Phys. Rev. B **25**, 4317 (1982); **26**, 3359 (1982).
[9]K.-M. Ho, C.-L. Fu, and B. Harmon, Phys. Rev. B **28**, 6687 (1983); **29**, 1575 (1984).
[10]J. Harris, R. O. Jones, and J. E. Muller, J. Chem. Phys. **75**, 3904 (1981); P. Bendt and A. Zunger, Phys. Rev. Lett. **50**, 1684 (1983).
[11]M. Weinert, E. Wimmer, and A. J. Freeman, Phys. Rev. B **26**, 4571 (1982).
[12]A. K. McMahan and John A. Moriarty, Phys. Rev. B **27**, 3235 (1983); M. Ross and A. K. McMahan, *ibid.* **26**, 4088 (1982); D. A. Young and M. Ross, *ibid.* **29**, 682 (1984), and references therein.
[13]M. Ross and A. K. McMahan, Phys. Rev. B **21**, 1658 (1980).
[14]A. Jayaraman, Rev. Mod. Phys. **55**, 65 (1983).
[15]D. M. Bylander and L. Kleinman, Phys. Rev. B **27**, 3152 (1983).
[16]A. Zunger and M. L. Cohen, Phys. Rev. B **19**, 568 (1979).
[17]H. J. F. Jansen and A. J. Freeman, Phys. Rev. B **30**, 561 (1984).
[18]E. Wimmer, H. Krakauer, M. Weinert, and A. J. Freeman, Phys. Rev. B **24**, 864 (1981).
[19]O. K. Andersen, Phys. Rev. B **12**, 3060 (1975); D. D. Koelling and G. O. Arbman, J. Phys. F **5**, 2041 (1975).
[20]D. R. Hamann, Phys. Rev. Lett. **42**, 662 (1979).
[21]D. D. Koelling and B. N. Harmon, J. Phys. C **10**, 3107 (1977).
[22]A. K. Rajagopal, J. Phys. C **11**, L943 (1978).
[23]A. H. MacDonald and S. H. Vosko, J. Phys. C **12**, 2977 (1979).
[24]E. Wigner, Phys. Rev. **46**, 1002 (1934).
[25]A. L. Altmann and A. P. Cracknell, Rev. Mod. Phys. **37**, 19 (1965).
[26]F. C. Von Der Lage and H. A. Bethe, Phys. Rev. **71**, 612 (1947).
[27]D. J. Chadi and M. L. Cohen, Phys. Rev. B **8**, 5747 (1973).
[28]R. W. G. Wyckoff, *Crystal Structure* (Wiley, New York, 1963), Vol. 1.
[29]F. D. Murnaghan, Proc. Natl. Acad. Sci. U.S.A. **30**, 244 (1944).
[30]Li-Chung Ming and Murli H. Manghnani, J. Appl. Phys. **49**, 208 (1978).
[31]P. W. Bridgman, Daedalus (Boston) **77**, 187 (1949).
[32]S. H. Chen and B. N. Brockhouse, Solid State Commun. **2**, 73 (1964).
[33]F. H. Featherstone and J. R. Neighbours, Phys. Rev. **130**, 1324 (1963).
[34]C. Kittel, in *Introduction to Solid State Physics,* 5th ed. (Wiley, New York, 1976), p. 74.
[35]L. Hedin and B. I. Lundqvist, J. Phys. C **4**, 2064 (1971).