PHYSICAL REVIEW B VOLUME 22, NUMBER 6 15 SEPTEMBER 1980

Investigation of the electronic properties of tellurium—energy-band structure

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(Received 12 October 1979)

The band structure of tellurium has been investigated by the orthogonalized plane-wave procedure using a Hartree-Fock-type potential, with a parameter introduced to incorporate consistency effects. The calculated band structure provides good agreement with a number of experimental results for energy differences involving the valence and conduction bands, obtained from reflectance measurements. The good agreement with experiment leads us to conclude that the electronic wave functions obtained from the present work are satisfactory. These wave functions are used in the following paper for a first-principles analysis of the ^{125}Te nuclear quadrupole interaction in tellurium.

I. INTRODUCTION

There has been considerable interest[1–3] recently in the nuclear quadrupole interaction of ^{125}Te in tellurium. The understanding of the origin of the nuclear quadrupole interaction of ^{125}Te in crystalline tellurium is of great interest because this interaction has been observed recently[1–3] in both crystalline and amorphous tellurium and also in selenium and sulfur. Thus ^{125}Te can be used as a probe to investigate the electronic distribution around the tellurium atom in different environments. With this aim in mind, in earlier work, we had attempted[4] to study the electron distribution associated with the tellurium atom and the corresponding ^{125}Te nuclear quadrupole interaction in tellurium, selenium, and sulfur using a semiempirical molecular orbital approach with clusters of large numbers of atoms to simulate the infinite atom environment in the solid. While such an analysis has been reasonably successful in explaining the absolute strengths of the nuclear quadrupole interaction and the trend of variation in going from tellurium to sulfur, it was felt that a more rigorous calculation in crystalline tellurium involving the electron distribution obtained from first-principles band-structure calculations would further enhance the understanding of the electronic structure of tellurium and also provide a test of the validity of the cluster-type analysis,[4] which, although semiempirical in nature, has the flexibility to be usable for both regular crystalline as well as noncrystalline environments.

With this aim in mind, we have carried out an investigation of the electronic structure of crystalline trigonal tellurium by the orthogonalized plane-wave procedure.[5] The reason for using the orthogonalized plane-wave (OPW) procedure is that electron densities using OPW wave functions have been found[6] to provide a successful explanation of the nuclear quadrupole interaction in a number of noncubic metals using recent developments[7] in the procedure for first-principles incorporation of antishielding effects in the calculation of field gradients in metals. The following paper will deal with the study of the field gradient in tellurium while the present paper is concerned with the band-structure investigation. We shall make comparisons between the predictions from our band-structure results and pertinent experimental data[8, 9] from reflection spectroscopy and ultraviolet photoemission measurements to obtain a test of the accuracy of the calculated band structure and hence indirectly of the associated wave functions. We shall also make comparisons of our OPW band-structure results with earlier results[10–17] by other procedures. Such a comparison is of interest not only because an OPW investigation of the band structure has not been attempted in the past, but also because we have used a different potential than that used in earlier[16] calculations, particularly with respect to exchange. For the exchange potential, we have avoided the use of the statistical exchange approximation[18] which has been found[19] to be inappropriate for study of hyperfine properties, involving the immediate vicinity of the nucleus where there is rapid variation in the electron distribution.

Among earlier band-structure investigations are those of Reitz[10] and Beissner[11] which employed the tight-binding and pseudopotential methods, respectively. Both these investigations were, however, restricted to the band structure along the Δ axis of the Brillouin zone (BZ) and hence could not address the question of the location of the band-gap minimum which has been considered to occur at the symmetry point H not covered in these calculations. Later, band-structure calculations employing the linear combination of atomic orbitals (LCAO),[12] Kohn-Korringa-Rostoker (KKR),[14] pseudopotential,[15] and modified augmented plane-wave (APW)[16] methods have been carried out along the Γ, Δ, S, and P symmetry axes. These calculations have all given broadly similar band structures for tellurium and with the exception of the APW calculation, were able to explain the location of band gap and its magnitude[20] reasonably well. The APW method gave the result that there are two band gaps of approximately the same magnitude at neighborhoods of the points H and Z, a result that has not been experimentally verified.

In Sec. II, the crystal structure and Brillouin zone of tellurium are briefly described. Section III describes the method of band-structure calculation including the calculation of the potential employed in this work. In Sec. IV our band-structure results are discussed and comparison is made with optical data and the results of earlier band calculations. Section V summarizes the main conclusions of our work.

II. CRYSTAL STRUCTURE AND BRILLOUIN ZONE OF TELLURIUM

The crystal structure of tellurium has been described in detail in the literature.[21] We present here a few details of the structure and Brillouin zone to facilitate the description of our band-structure calculations. In the tellurium lattice, the atoms are arranged on spiral or helical chains at the center and corners of a regular hexagon. The chains have a threefold screw axis corresponding to the crystal c axis, and the unit cell has three atoms whose positions using a rectangular coordinate system are given by:

$$\vec{\tau}_1 = -ua\,\vec{i}\ , \tag{1}$$

$$\vec{\tau}_2 = \tfrac{1}{2}ua\,\vec{i} - (\tfrac{1}{2}\sqrt{3})ua\,\vec{j} + \tfrac{1}{3}c\,\vec{k}\ , \tag{2}$$

$$\vec{\tau}_3 = \tfrac{1}{2}ua\,\vec{i} + (\tfrac{1}{2}\sqrt{3})ua\,\vec{j} + \tfrac{2}{3}c\,\vec{k}\ . \tag{3}$$

All the atoms in the entire crystal can hence be generated from these three atoms by adding a lattice translation vector $\vec{R}$, defined by

$$\vec{R} = l\,\vec{t}_1 + m\,\vec{t}_2 + n\,\vec{t}_3\ , \tag{4}$$

where l, m, n are integers and $\vec{t}_1$, $\vec{t}_2$, $\vec{t}_3$ are the primitive lattice vectors defined by

$$\vec{t}_1 = -\tfrac{1}{2}a\,\vec{i} - a\tfrac{1}{2}\sqrt{3}\,\vec{j}\ , \tag{5}$$

$$\vec{t}_2 = a\,\vec{i}\ , \tag{6}$$

$$\vec{t}_3 = c\,\vec{k}\ . \tag{7}$$

In the above equation, $\vec{i}$, $\vec{j}$, $\vec{k}$ are the orthogonal unit vectors defining x, y, and z direction, respectively, a, c, and u are lattice parameters whose values are 4.4572, 5.929, and 0.2633 Å, respectively,[22] at 298 K and standard pressure and are the values used in our present work. The basis vectors $\vec{b}_i$ in the reciprocal space which determine the Brillouin zone are given by

$$\vec{b}_1 = \frac{-4\pi}{a\sqrt{3}}\vec{j}\ , \tag{8}$$

$$\vec{b}_2 = \frac{2\pi}{a}\vec{i} \frac{-2\pi}{a\sqrt{3}}\vec{j}\ , \tag{9}$$

$$\vec{b}_3 = \frac{2\pi}{c}\vec{k}\ . \tag{10}$$

The Brillouin zone of tellurium, which is hexagonal, is shown in Fig. 1. The irreducible wedge, respresenting $\frac{1}{12}$ of the Brillouin-zone volume, for the calculation of properties requiring the knowledge of the wave functions is shown in Fig. 2. More de-

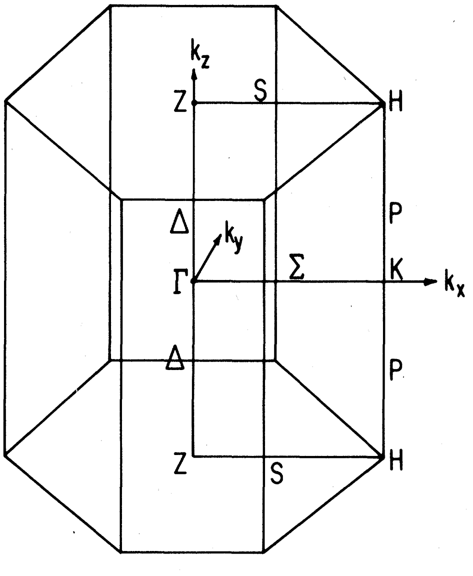

FIG. 1. Brillouin zone of tellurium showing symmetry points and symmetry lines.

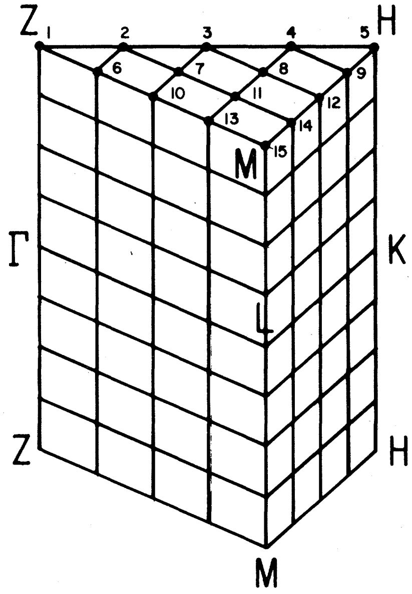

FIG. 2. Irreducible wedge corresponding to $\frac{1}{12}$ Brillouin zone used in the band calculations.

tails about the symmetry properties of tellurium can be found in the earlier literature.[23]

III. PROCEDURE

For obtaining the energy bands and Bloch wave functions for the system, we have to solve the one-electron Schrödinger equation given by

$$H\psi_{\vec{k}}(\vec{r}) = E_{\vec{k}}\psi_{\vec{k}}(\vec{r}) \ . \tag{11}$$

There are only a few instances in the literature, where self-consistent Hartree-Fock calculations, with or without correlation have been carried out. Among these are calculations in very simple metals such as alkali metals,[24,25] especially lithium and the ferromagnetic transition metals,[26] iron, cobalt, and nickel. More often, one makes a local approximation[27] to the exchange interaction, including the Slater-type free-electron approximation[18] that has often been employed. For the local approximation one can write, using Rydberg units,

$$H = -\nabla^2 + V(\vec{r}) \ , \tag{12}$$

where the potential

$$V(\vec{r}) = \sum_{i=1}^{N}\sum_{\nu=1}^{3} v(|\vec{r} - \vec{R}_i - \vec{\tau}_{i\nu}|) \tag{13}$$

is periodic in the crystal lattice, $\vec{R}_i$ representing the position of the center of the ith unit cell and $\vec{\tau}_{i\nu}$ the position of the νth atom in the unit cell with respect to the center of the ith cell, there being three atoms in the unit cell in tellurium. We shall discuss the form of the potential we have used subsequently in this section.

For the sake of completeness, we shall first briefly review the OPW procedure used in our work. The basis set for the variational solution of Eq. (11) in the OPW procedure is of the form:

$$F_{\mathrm{OPW}}(\vec{k}, \vec{r}) = \frac{1}{(N\Omega_0)^{1/2}} \exp(i\vec{k}\cdot\vec{r}) - \sum_j \mu_{\vec{k}j}\phi_{\vec{k}j}(\vec{r}) \ , \tag{14}$$

where Ω_0 is the volume per atom and N is the number of atoms in the lattice, while the $\phi_{\vec{k}j}(\vec{r})$ are tight-binding core wave functions given by

$$\phi_{\vec{k},j}(\vec{r}) = \frac{1}{(3N)^{1/2}} \sum_{i=1}^{N}\sum_{\nu=1}^{3} e^{i\vec{k}\cdot\vec{R}_i} e^{i\vec{k}\cdot\vec{\tau}_{i\nu}} \phi_j(\vec{r} - \vec{\tau}_{i\nu}) \ . \tag{15}$$

In Eq. (15), $\phi_j(\vec{r} - \vec{\tau}_{i\nu})$ represents the jth atomic core wave function centered at the position of the νth site in the ith unit cell. The summation over j runs over all the cores 1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, and 4d in tellurium, the 5s and 5p electrons being handled as band electrons. The quantities $\mu_{\vec{k}j}$ in Eq. (14) refer as usual to the orthogonalization parameters given by

$$\mu_{\vec{k},j} = \left[\frac{3}{\Omega_0}\right]^{1/2} \int e^{i\vec{k}\cdot\vec{r}}\phi_j(\vec{r})\, d^3r \ . \tag{16}$$

In the secular equation

$$\mathrm{Det}|H_{mn} - ES_{mn}| = 0 \tag{17}$$

obtained by minimizing the energy with respect to the coefficients $c(\vec{k} + \vec{K}_n)$ in the linear combination of OPW functions

$$\psi_{\vec{k}}(\vec{r}) = \sum_n c(\vec{k} + \vec{K}_n) F_{\mathrm{OPW}}(\vec{k} + \vec{K}_n, \vec{r}) \ , \tag{18}$$

the matrix elements of the Hamiltonian are given by

$$H_{mn} = \langle F_{\mathrm{OPW}}(\vec{k} + \vec{K}_m, \vec{r})| -\nabla^2 + V(\vec{r})|F_{\mathrm{OPW}}(\vec{k} + \vec{K}_n, \vec{r})\rangle \ . \tag{19}$$

In view of the form of the OPW functions in Eq. (14), the matrix elements H_{mn} in Eq. (19) involve component matrix elements such as $\langle A|-\nabla^2 + V(r)|B\rangle$ where A and B can both be plane waves, or both be tight-binding core functions, or, either A or B can be a plane wave and the other a tight-binding core function, referred to, respectively, as PW-PW, core-core, and PW-core terms. The latter two types of terms involving the core states can be substantially simplified[27] using

$$[-\nabla^2 + V(\vec{r})]\phi_{\vec{k}j}(\vec{r}) = \epsilon_j\phi_{\vec{k}j}(\vec{r}) \ , \tag{20}$$

where ϵ_j are core-state energies. These were taken to be the same as those in the atom, since the differences of these energies from those in the solid state due to differences in the potentials seen in the two cases have been found to be quite small in transition metals,[28] and these differences are expected to be comparable in importance or even smaller for a tightly-bound system involving s and p band electrons as in the present case. The overlap integral S_{mn} is given by

$$S_{mn} = \langle F_{\mathrm{OPW}}(\vec{k} + \vec{K}_m, \vec{r})|1|F_{\mathrm{OPW}}(\vec{k} + \vec{K}_n, \vec{r})\rangle \ . \tag{21}$$

We shall discuss next our choice for the potential $v(r)$. Ideally, one would like to use a potential as close to first principles as possible. As pointed out earlier, the best way to do this is to use the rigorous Hartree-Fock approach,[24–26] recognizing completely the nonlocal nature of the exchange and not look for an $\vec{r}$-dependent potential but rather work directly with the matrix elements of the multielectron Hamiltonian of the system. Such a process is very satisfactory from a theoretical point of view but rather time consuming. A simpler approximation would be to use for the potential a combination of the actual Coulomb potential due to the conduction and core electrons and the statistical free-electron approximation[18] for the contribution of exchange interactions to the potential. While this approximation is rather simple and speedy for computational purposes and also provides reasonably accurate energy-band results,[29] it leads to inaccuracies in the wave functions, especially in the neighborhood of the nucleus,[19] where the charge distribution does not satisfy the criterion of smooth and slow variation necessary for the validity of the free-electron-like statistical approximation for exchange. Unfortunately, the region near the nucleus is the one we are most interested in for hyperfine properties. A good compromise in terms of accuracy of the wave functions and economy of effort is to use a local potential based on Hartree-Fock exchange as has been done in some instances earlier[27] in the literature. In contrast to good metals, where the free-electron approximation is reasonable, in tellurium one expects the wave functions to be more localized in nature. This was indeed found to be the case from our calculation since a sizable number of OPW functions were needed to obtain convergence in the energy and wave functions in this system. In view of this, a superposition of atomic Hartree-Fock potentials at the lattice sites was expected to be a reasonable choice for the potential in the solid. The potential we have used is given by Eq. (13) with

$$v(r)=\begin{cases}V_a(r)+V_0, & r\leq r_{\mathrm{WS}},\\ 0, & r>r_{\mathrm{WS}},\end{cases} \tag{22}$$

r_{WS} being the radius of the Wigner-Seitz sphere around each atom and $V_a(r)$ a weighted admixture of the one-electron Hartree-Fock potentials:

$$v_{5s}(r_1)=\sum_j\left\langle\phi_j(r_2)\left|\frac{1}{r_{12}}\right|\phi_j(r_2)\right\rangle - \sum_j\left\langle\phi_j(r_2)\left|\frac{1}{r_{12}}\right|\phi_j(r_2)\right\rangle\frac{\phi_j(r_1)}{\phi_{5s}(r_1)}\ , \tag{23}$$

$$v_{5p}(r_1)=\sum_j\left\langle\phi_j(r_2)\left|\frac{1}{r_{12}}\right|\phi_j(r_2)\right\rangle - \sum_j\left\langle\phi_j(r_2)\left|\frac{1}{r_{12}}\right|\phi_j(r_2)\right\rangle\frac{\phi_j(r_1)}{\phi_{5p}(r_1)}\ , \tag{24}$$

where j runs over all the cores $1s$, $2s$, $2p$, $3s$, $3p$, $3d$, $4s$, $4p$, $4d$, and $5s$ and $5p$ electrons in the valence shells of the tellurium atom. Thus v_{5s} and v_{5p} represent, respectively, the potential seen by the $5s$ and $5p$ electrons in tellurium atom. It was found that $v_{5s}(r)$ and $v_{5p}(r)$ were quite close to each other. Consequently the exact fractional weights assigned to $v_{5s}(r)$ and $v_{5p}(r)$ were not too crucial. The fractional

TABLE I. Comparison bewtween transition energies from present work, experiment, and earlier calculations (in eV).

	Expt.[a]	OPW[b]	APW[c]	KKR[d]	Pseudopotential[e]	Pseudopotential[f]
Gap transition energy close to s axis	1.75	1.5				
Energy difference between lowest and next lowest conduction band at H	1.3	1.41	0.6	0.69	0.94	1.07
Threshold for transition energy between the second highest valence band triplet and the lowest conduction band	4.0	5.62	3.0	1.86		4.8
Transition energy from the top of the valence band to the top of the lowest conduction band	2.3	1.77	2.5	1.0	1.36	1.6
Energy differences between the bottom of the conduction band K_3^4 at K and the following points						
(i) Γ_2^2	1.6	1.05	2.04	1.79	1.61	1.85
(ii) H_1^2		1.71	0.7	1.30	1.85	2.5
(iii) Z_1^2		1.22	1.65	1.72	1.98	2.25

[a] Reference 8.
[b] Present work.
[c] Reference 16.
[d] Reference 14.
[e] Reference 15.
[f] Reference 17.

weighting factors we choose are 33% and 67% for $v_{5s}(r)$ and $v_{5p}(r)$, respectively. The parameter V_0 in Eq. (22) was introduced for the following reasons. For a rigorous first-principles calculation, one has to incorporate self-consistency in the potential experienced by the band electrons (both valence and conduction bands, if one is interested in transition energies) and many-body effects arising from dynamic correlation between the electrons. As mentioned earlier above, such effects have been incorporated in a first-principles way in the literature for only a few relatively simple metals. Such a procedure would be beyond the scope of the present work. We have instead attempted to incorporate these effects indirectly through the empirical parameter V_0. The influence of consistency effects is not expected to affect the core-conduction Coulomb and exchange components of the potential significantly, since the Coulomb interactions involve only the core electron functions which do not change appreciably from the free atom to the solid, the core-conduction exchange terms involving the conduction-electron wave function also being relatively unaffected by consistency effects since the differences between Bloch functions for the band electrons and the 5*s* and 5*p* wave functions in Eqs. (23) and (24) are not significant in the internal regions of the atom. The influence of correlation effects between core electrons and conduction electrons is also not expected to be pronounced because it is like an intershell effect which has been found to be relatively unimportant from explicit calculations in atomic systems.[30] So whatever influence consistency and correlation effects have is associated with the interaction among band electrons. We have attempted to incorporate them through the parameter V_0 by adjusting the latter to fit the experimentally derived value of 0.34 eV for the fundamental band gap[20] which occurs at the H point of the Brillouin zone. The value obtained for V_0 in this way was 0.36 eV which is a reasonable order of magnitude. The adequacy of this parameter was confirmed from comparison of theory and experiment for a number of features of the valence and conduction bands in Table I to be discussed in Sec. IV. The convergence of our calculation of the band energies, with respect to the number of OPW functions used in Eq. (18) are discussed in the next section where our band-structure results are presented.

IV. RESULTS AND DISCUSSION

The convergence of our band calculations was studied by examining the energies at typical points in the Brillouin-zone wedge in Fig. 2, as a function of the number of OPW functions. In choosing the number of OPW functions, especially at symmetry points, all vectors $\vec{k}+\vec{K}$ having the same length were included so as to retain the proper symmetry at these points. The convergence criterion for energy was 0.01 eV, typically 55 and 54 OPW, respectively, being needed at symmetry points Γ and Z to reach the chosen convergence limit. At general points with low symmetry, usually about 60 OPW were needed to reach the required convergence criterion.

The energy bands obtained from our calculation are shown in Fig. 3. The first nine bands constitute the valence bands that accomodate the 18 valence electrons arising from six valence electrons in each of the three atoms in the unit cell. The next three bands represent the triplet of conduction bands. Our calculated band structure, in terms of the overall arrangement of, and separations between, the bands agree reasonably well with previous[14–17] band calculations, most of which have been nonrelativistic in nature like the present investigation. Since the methods of calculation are rather different for the various available band structures including our present one, it is not very meaningful to make detailed comparisons at various points in the Brillouin zone between the bands obtained from different calculations. It is instead more enlightening to make comparisons with respect to specific energy-band gaps and energy differences that are available from experimental measurements. We shall discuss this shortly, but before that, to obtain a perspective of the overall relationship between the band structures from different calculations, we would like to briefly remark on some special points of agreement and difference between our band structure and some of the others, some examples of which will now be quoted. Thus, in the ΓZ direction, our band-structure results are in better agreement with those from APW[16] and recent pseudopotential[17] calculations than with those from earlier KKR[14] and pseudopotential[15] work. For instance, for the lowest valence band triplet, our results show that at the Γ point and all through the line ΓZ, a Δ_1 level is the lowest one, in agreement with the APW[16] and recent pseudopotential[17] calculations. The lowest valence band is not available for the KKR[14] and earlier pseudopotential[15] calculations. For the second triplet of valence bands, there is greater similarity in our level arrangement with the results of APW and recent pseudopotential calculations than with the KKR results.[14]

In the HK direction, our arrangement of the energy bands is in satisfactory agreement for the first, third, and fourth band triplets with those from the APW[16] and recent pseudopotential[17] calculations as well as the KKR[14] and earlier pseudopotential[15] calculations, only the second, third, and fourth triplets being available in the KKR calculation and the third and fourth in the earlier pseudopotential work. There are differences in detail in the slopes of the bands for the second triplet of levels between our work and others.

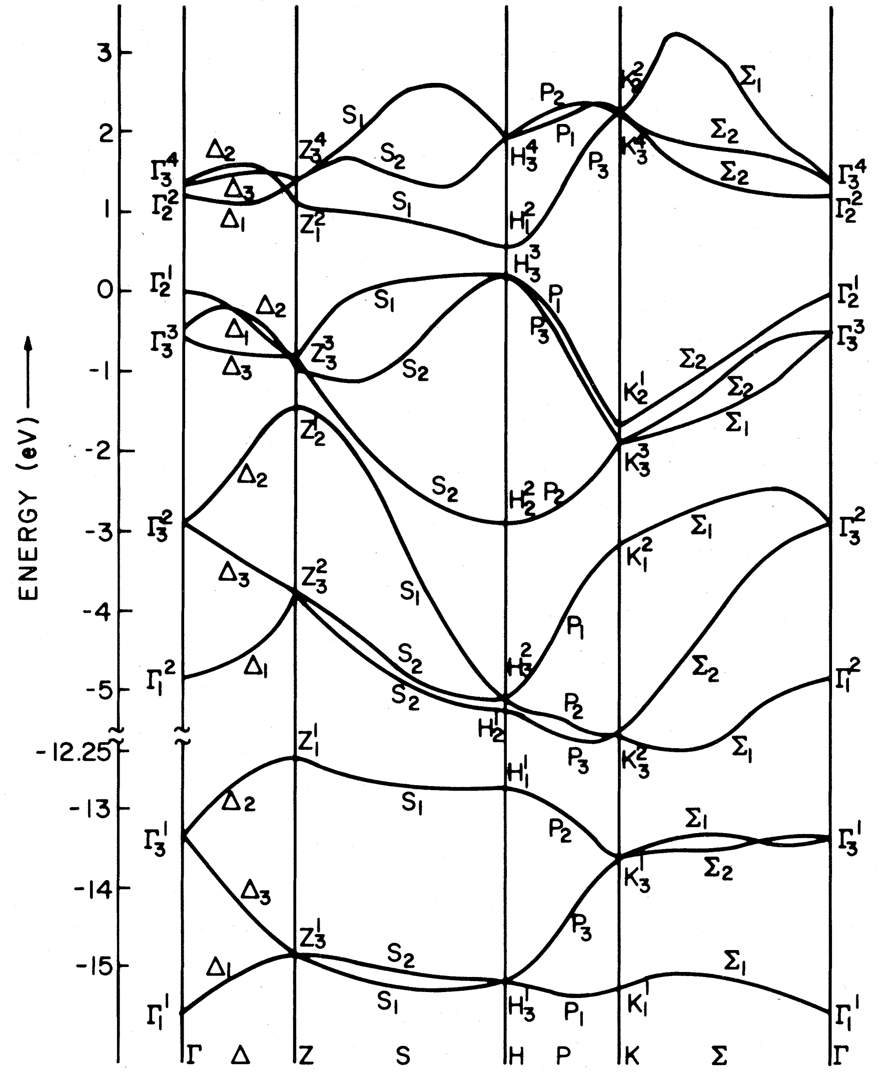

FIG. 3. Energy bands of tellurium.

In the other directions where results of earlier band calculations are available to compare with our results, there appears to be overall agreement between our results and those of the other calculations excluding the APW calculation for which results are not available from other directions besides ΓZ and HK. The agreement with the recent pseudopotential calculations is in general somewhat closer than with the KKR and earlier pseudopotential results.

A more specific comparison between the results of our band calculation and those of other calculations and experiments can be made by considering features of the energy bands that are available from recent analysis of reflection spectra.[8] We have already used the band gap between the bottom of the conduction band and the top of the valence band at *H* for obtaining the parameter V_0 in the potential in Eq. (22). We shall make a comparison for the other transition energies that have been measured. In the first row of Table I, we have compared the gap transition energy represented by the energy difference between the two adjacent S_2 levels of the highest occupied triplet of band states in the neighborhood of the middle of the *ZH* line. The next row represents the difference in energy between the lowest conduction band at *H* and the next higher one. The third row corresponds to the threshold energy for the transition between second highest valence-band triplet and the conduction band. From our band-structure results, the proper quantity to compare this threshold energy with is the energy difference between the second valence-band triplet of states at the *H* point and the bottom of the lowest conduction band at this point. The next row represents the energy of transition from the top of the valence band to the maximum of the lowest conduction band. From our band-structure results in Table I, the appropriate energy difference to compare this with is that between H_3^3 in the valence band and K_3^4 in the conduction band. The final set of three rows represents the energy differences between the lowest conduction-band energy at the K point and the corresponding energy for the Γ, H, and Z points. Only the average of these three energies is available from experiment for comparison.

The agreement between our results for energy differences in Table I and those from other procedures follows the pattern found from the comparison of the band structures made earlier. Thus, overall, there is better agreement between our results and those from recent pseudopotential calculations and to a lesser extent, the APW work than those from the KKR and earlier pseudopotential calculations.

Comparing our results with experiment, we find that there is good agreement with all the transition energies listed, the agreement being most satisfactory for the first two gaps, in Table I. The agreement with experiment is overall more satisfactory than is the case for the APW procedure[16] which also employs a real potential as is done in the present calculation. Thus, while the agreement between APW results and experiment is comparable for the last four transition energies in Table I, for the second gap corresponding to the energy difference between the lowest and next lowest conduction band at H, the APW result is only about one half of the experimental result while the OPW result in the present work is in good agreement with experiment. Among the probable reasons for the somewhat better agreement with experiment by our OPW calculation is the difference in the procedures used for the band calculations in the two cases and the difference in the potentials used. The latter reason is perhaps more likely, since the valence wave functions in tellurium appear to be localized in nature, leading to a departure from the smoothness condition necessary for the validity of the Slater exchange approximation[18] employed for the potential used for the APW calculation.

The good agreement between the results of the OPW calculation for the band-structure dependent properties in Table I and experiment also indicates the appropriateness of choice of the form of the potential in Eq. (22) involving the parameter V_0 for inclusion of correlation and consistency effects in both the valence and low-lying conduction bands. It is satisfying that while V_0 was obtained by adjusting the band gap at one $\vec{k}$ point, one has obtained good agreement over a number of different $\vec{k}$ points. This indicates that the energy bands and wave functions are satisfactory over the entire Brillouin zone, a fact that is important for the study of the electric field gradient at the nucleus contributed to by all the valence-band electrons. It would be desirable in future work to obviate the need for this parameter V_0 by carrying out a self-consistent calculation of the band structure, using the calculated band wave functions to obtain a new potential and carrying out the process iteratively towards convergence. This would be a rather time-consuming procedure but it would be interesting to see if one is able to obtain, by such a process, a comparable agreement with experiment as obtained in the present work using the adjusted parameter V_0 in the potential.

V. CONCLUSION

In summary, the OPW calculation in the present work has provided satisfactory agreement with the experimentally observed features of the band structure. This satisfactory agreement, and the fact that a potential has been used that is expected to be valid over the entire Wigner-Seitz cell including the region in the neighborhood of the nucleus where the electron density is rapidly varying, leads one to expect that the wave functions obtained from the present calculations would be suitable for analysis of magnetic and nuclear quadrupole hyperfine interactions.

ACKNOWLEDGMENT

This work was supported by the National Science Foundation.

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