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# Calculation of elastic constants in UC, US, and UTe

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The calculated electronic structure and charge density of UC and US are reported. We also report calculations on the elastic constants of the cubic compounds UC, US, and UTe using the local-spin-density approximation (LSDA) to the exchange and correlation potential. Good agreement between calculations and experiment has been obtained for UC and US suggesting that the chemical bonding is well reproduced by LSDA for these two compounds. In contrast, for UTe the calculations do not reproduce the measured negative Poissons ratio (negative $C_{12}$). We suggest that the failure to describe the elasticity of UTe reflects the weakness of LSDA in describing accurately electron systems that are strongly correlated and we speculate that UTe is an anomalous, possibly mixed valent, system.

## I. INTRODUCTION

Uranium forms NaCl-type 1:1 compounds with many of the $p$ elements.[1] The physical properties of these compounds vary substantially depending upon the anion. The present paper is mainly devoted to the study of elastic constants and interatomic forces for these systems and in our investigation, we have selected three compounds, UC, US, and UTe, for reasons which will become clear below. UC is believed to be an itinerant $5f$-electron system with relatively broad $f$ bands. Consequently, the influence of the $5f$ electrons on the cohesive properties is expected to be large. Due to a combination of the smallness of the C atom and the itinerant (and therefore bonding) $5f$ states of the U atom, the unit cell volume is quite low, and the bulk modulus is correspondingly high. Energy band calculations,[2,3] in which the $5f$ electrons were assumed to be itinerant, reproduced the equilibrium volume and the bulk modulus of UC within a few percent. These calculations[2,3] also suggest that UC should be a Pauli paramagnet, since it was also demonstrated that the $5f$ band was relatively broad in UC and that the Fermi energy ($E_F$) was situated in a region where the state density, $N(E)$, was low. The effective Stoner parameter, $I$, was calculated to be 0.46 eV and the calculated state density per spin at the Fermi energy 1.1 per eV per formula unit. This gives a Stoner product, $IN(E_F)$, which is only 0.52 and, therefore, only a moderately enhanced paramagnetic susceptibility is expected. The experimentally observed temperature independent paramagnetism of UC could, therefore, be understood from the calculated Stoner product.

Moreover, calculations of the Fermi surface of UC (Refs. 4 and 5) agree well with experimental data.[6] The Fermi surface, which is similar to that of ThC,[4] consists of two hole ellipsoids centered at $X$ and an electron sheet centered at $W$. The calculated extremal areas and masses on the three sheets in UC are in reasonable agreement with dHvA experiments,[6] indicating the presence of $5f$ states at the Fermi energy. If the $5f$ states had not been included in the band structure calculations, the calculated Fermi surface would not have been in agreement with the measurements. The presence of an itinerant $5f$ band pinned at the Fermi energy may also, if perhaps less unambiguously, be deduced from the relatively large linear specific heat constant, $\gamma$, which is $\sim 20.3\ \mathrm{mJ/mol\,K^2}$.[7] We believe, therefore, that UC is a $5f$-band Pauli paramagnet.

The presence of $5f$ states at $E_F$ in US is also indicated by the electronic specific heat constant, $\gamma$, which is $23.3\ \mathrm{mJ/mol\,K^2}$.[7] The photoemission spectrum shows a strong $5f$ peak at $E_F$ and it was concluded[8] that optical spectra from this compound lack "fingerprints" of any localized $5f^n$ configuration. Also, from optical and magneto-optical measurements, Reim and Schoenes[9] concluded that the $6d$ occupation is 1.1 and the $5f$ occupation is 2.9. From the absence of any fine structure and the width of the $f \to t_{2g}$ transition together with the large $d$-$f$ oscillator strength, Schoenes also argued that the degree of delocalization of the $5f$ states in US is substantial. However, he also pointed out difficulties in explaining electrical and optical conductivity data using itinerant $5f$ states.

Another indication that the $5f$ states in US are delocalized was given by energy band calculations,[10] which reproduced the experimental equilibrium volume of US within a few percent. The calculated bulk modulus did not appear to be in good agreement with measurements available at the time, but subsequent experiments have tended to converge towards the theory.[11–28] Furthermore, US is ferromagnetic below 177 K and, among the NaCl-type ferromagnets, has the smallest lattice constant. The nature of the magnetism in US is not fully understood and is a very interesting problem. The total magnetic moment at low temperatures has been measured to be $\sim 1.55\mu_B$,[29,30] whereas the $5f$ contribution to the moment, determined by neutron diffraction, is $1.7\mu_B$.[30] The difference of $-0.15\mu_B$ is due to the diffuse conduction electrons polarized *antiparallel* to the total moment. That the "*spd*" (mostly $6d$ in U compounds) diffuse electron spin moment is observed to be antiparallel to the total moment is confirmed by spin-polarized photoemission experiments on uranium chalcogenides [31] and deduced from magneto-optical measurements.[9] However, the calculated diffuse moment is always parallel to the total *spin* moment in actinide NaCl-type compounds. Only if the orbital component of the moment at the uranium site is larger than, and antiparallel to, the spin component can theory and experiment be consistent. Then the sign of the total moment is determined by the orbital component. This situation is consistent with all known data.

Conventional self-consistent spin-polarized energy band calculations, with the spin-orbit coupling omitted,[32] result in a spin moment of about $2\mu_B$ in US. Self-consistent relativistic energy band calculations yield a large orbital contribution to the magnetic moment antiparallel to, and larger in magnitude than, the spin contribution.[32] Attempts to obtain the correct magnitude of the spin and orbital moments in US have been reasonably successful.[32,33] For instance, the magnetic moment of US was calculated by Severin *et al.*,[33] who showed that using itinerant states in combination with an orbital polarization corrected LSDA formalism (LSDA+OP), the magnetic moments (spin and orbital) of US could be accounted for. There is now ample evidence that US has, although it is cubic, an enormous magnetic anisotropy at low temperatures. The energy difference obtained with the magnetic moment aligned along the [001] and [111] directions of US was calculated by Brooks *et al.*[34] to be extremely large, of the order of $10^{10}$ ergs/cm$^3$. The magnetic easy axis was calculated to be in the [111] direction, in agreement with measurements. Lander *et al.*,[35] measured this quantity and found it to be about half of the calculated value. Under pressure, the Curie temperature decreases with $-0.23$ K/kbar.[36] This and all the results quoted above seem to support an itinerant $5f$ model in US. The $5f$ states are thus expected to be chemically bonding in US, but to a lesser degree than in UC.

In UTe the $5f$ bonding is expected to be smaller than in US, partly due to the fact that among the three materials studied presently, this is the system with the largest anion. This compound is a ferromagnet below 104 K with the easy axis in the [111] direction and with a moment of $2.25\mu_B$. Although not as thoroughly studied theoretically as US, the lattice constant and bulk modulus have been calculated[10] and spin-polarized energy band calculations[32] yield approximately the correct measured total moment when all relativistic effects are included. The remarks made above for US concerning the relative signs of the spin, orbital, and diffuse moments also apply to UTe. There are, however, indications from experiment that the nature of the magnetism may be quite different in UTe. First, the calculated bulk modulus[10] is twice the measured value, an exceptional anomaly for uranium NaCl-type compounds. The measured electronic specific heat constant of UTe (Ref. 37) is $\sim 10$ mJ/mol K$^2$, whereas the calculated state density at the Fermi energy is actually larger than in US. The Curie temperature increases under pressure up to 5 GPa, after which it decreases — as in US.[38] This type of behavior is reminiscent of a suppression of the Kondo reduction of the moment below 5 GPa,[39] after which the negative pressure derivative is indicative of an itinerant electron system. Actually, magnetic excitations are observed in UTe,[16] whereas there is no sharp response in US. Finally, the elastic constants are anomalous in UTe — the Poisson ratio being negative, whereas it is positive in UC and US.[20,21]

For our present study, we have thus selected three compounds with varying degree of $5f$ bonding. Clearly this rather pronounced difference is expected to be reflected in the elastic properties. For instance, the bulk modulus is largest in UC and smallest in UTe, whereas the equilibrium volumes display the opposite trend. These differences cannot be attributed to a difference between the $5f$ behavior unless we can quantify these differences. Further, the elastic constants ($C_{11}$, $C_{12}$, and $C_{44}$) are smaller for the systems with larger volumes and, most interestingly, in US the $C_{12}$ constant is only slightly positive, whereas for UTe it is negative. A negative $C_{12}$ is quite common for intermediate valence systems and its occurrence seems to be connected to a very low bulk modulus $B$. To illustrate this we observe that one can write, $C_{12} = B - \frac{2}{3}C'$, where $C'$ is the so-called tetragonal shear constant. The size of $C'$ reflects the degree of stability of the crystal with respect to a tetragonal shear and a negative $C_{12}$ thus means that it costs more in energy to distort the crystal structure (in a tetragonal way) than to modify the volume. The trends of the observed elastic constants of the above-mentioned compounds have motivated us to study them theoretically by means of first principles calculations. The rest of this paper is organized as follows. In Sec. II, we describe the details of the computational method. In Sec. III, we describe the result of the present calculations and in Sec. IV, we present our conclusions.

## II. COMPUTATIONAL DETAILS

In the present electron structure calculations, we use a full-potential linear muffin-tin-orbital technique.[40] The calculations were all electron, fully relativistic with the spin-orbit coupling included at each variational step.[41] Furthermore, no shape approximation to the charge density or potential was used. The exchange and correlation part of the potential was treated in the local-spin-density approximation (LSDA), using the von Barth–Hedin expression[42] for the exchange-correlation functional. The base geometry consists of a muffin-tin part and an interstitial part. Inside the muffin-tin part the basis functions, charge density, and potential were expanded in a spherical-harmonic series and in a Fourier series in the interstitial. The spherical-harmonic expansion of the charge density, potential, and basis functions were carried out to $l$=8. The basis set was comprised of augmented linear muffin-tin orbitals.[41,43] The tails of the basis functions outside their parent spheres were linear combinations of Hankel or Neuman functions with nonzero kinetic energy $\kappa^2$ (the kinetic energy of the basis functions in the interstitial region). The basis included 6*p*, 7*s*, 7*p*, 6*d*, and 5*f* partial waves on the uranium (cation) site and *s*, *p*, and *d* orbitals for the anion site. Further, for the uranium site all orbitals were contained in the same energy panel, with the 6*p* states treated as pseudovalence states calculated at a different energy, $\epsilon_\nu$, than for the rest of the basis functions. Further, we adopted a so-called "double basis," where we used two different partial waves of $l,m_l$ character each connecting, in a continuous and differentiable way, to Hankel or Neuman functions with different kinetic energy $\kappa^2$. We used three sets of tail parameters, including two tails in each set, with one set for the U 6*p* states, and one set for the valence states. The tails used here range from −2.1 to 0.8 Ry. The integration over the Brillouin zone was done using the special point sampling[44] with a Gaussian smearing width of 10 mRyd. The number of *k* points was increased until the change in the total energy was less than 0.5 mRyd. Thus, to ensure convergence in **k** space, we found it necessary to use 275 *k* points in the 1/16th Brillouin zone for the tetragonal shear ($C'$) and 288 *k* points in the 1/8th Brillouin zone for the orthorhombic shear ($C_{44}$). The calculations of the elastic constants were done at the calculated equilibrium volume and the volume ratio between the interstitial region and the unit cell was approximately 0.5 in these calculations.

## III. RESULTS

### A. Elastic constants

The calculated elastic constants for UC are compared to experimental data in Table I. Notice that the agreement between theory and experiment for this material is between ∼6% and ∼11%. The calculations overestimate the bulk modulus, Table II (a common feature of calculations based on the local density approximation), and the $C_{11}$ constant. For the $C_{12}$ and $C_{44}$ constants, the agreement is very good. The results, presented in Table I, show equally good agreement with experiment as those obtained from similar calculations for the transition metals.[45] This shows that from this point of view, LSDA calculations are quite successful for UC. In Table II, we compare the calculated equilibrium volume, bulk modulus, and tetragonal shear constant with experimental values for UC, US, and UTe. It should be noted here that the calculations for US and UTe were spin polarized. The resulting spin and orbital moments for US were $1.81\mu_B$ and $-2.08\mu_B$, respectively. For UTe, the moments were $1.84\mu_B$ and $-2.38\mu_B$, respectively. From Table II, it is clear that the calculated equilibrium volumes agree within ∼ 10% for all three compounds. For UC and US, the agreement is fairly good concerning the bulk modulus and the tetragonal shear constant and again the error made in these calculations is comparable to what one makes for the transition metals (particularly the early ones such as vanadium[45,46]). In contrast, for UTe our calculations fail to reproduce the experimental data for $B$ and $C'$. For this compound, the calculated bulk modulus is more than a factor of 3 too large and the calculated tetragonal shear constant is ∼ 72% too large.

TABLE I. Experimental (Ref. 49) and calculated elastic constants for UC at the equilibrium volume.

| | Elastic constant (GPa) | | |
|---|---|---|---|
| | $C_{11}$ | $C_{12}$ | $C_{44}$ |
| Theory | 350 | 79 | 65 |
| Experiment | 315 | 77 | 61 |

We have also performed additional calculations for US using the orbital polarization correction to the local spin density functional, in the way suggested by Eriksson *et al.*[47] The so calculated uranium 5*f* spin moment is $-1.65\mu_B$ and the uranium 5*f* orbital moment is $3.11\mu_B$. The total spin moment of the cell (including diffuse magnetization) is −1.99 and the total moment is thus $1.12\mu_B$ per cell. Experimentally, the 5*f* spin moment is $-1.3\mu_B$, the 5*f* orbital moment is $3.0\mu_B$, and the total moment is $1.55\mu_B$ per cell. It, thus, seems that our calculations overestimate the 5*f* spin moment by $0.35\mu_B$, whereas the calculated orbital moment agrees better with experiment. The calculated diffuse moment is $-0.25\mu_B$, to be compared to the experimental value of $-0.15\mu_B$. In Table II, we compare the equilibrium volume, tetragonal shear constant, and bulk modulus for the LSDA, and LSDA+OP calculations. Note that there is very little difference between the calculated equilibrium volumes. However, the shear constant is slightly higher for the LSDA+OP then for the LSDA calculation. As regards the bulk modulus, the LSDA calculation agrees slightly better with experiment.

From the discussion above, it would seem that when comparing the theoretical and experimental equilibrium volumes, the agreement is acceptable for all three compounds, whereas concerning the bulk modulus and the tetragonal shear constant, there is good agreement only for UC and US. The failure to reproduce the experimental bulk modulus for UTe suggests a failure of the local density approximation and is consistent with the analysis of Mendik and Wachter,[48] who state that UTe is a mixed valence system. An interesting aspect of the elasticity is that systems, which have a negative $C_{12}$ normally, also have an intermediate valence,[48] and UTe might be an ex-

TABLE II. Experimental (Ref. 49) and calculated equilibrium volume, tetragonal shear constant, bulk modulus at the calculated equilibrium volume for UC, US, and UTe.

| | Theory | | | | Experiment | | |
|---|---|---|---|---|---|---|---|
| | UC | US (LSDA) | (LSDA+OP) | UTe | UC | US | UTe |
| Equilibrium volume $V_0$ (Å) | 27.15 | 37.26 | 38.40 | 52.54 | 30.51 | 41.34 | 58.29 |
| $C'$ (GPa) | 137 | 140 | 160 | 141 | 118 | 144 | 82 |
| Bulk modulus (GPa) | 168 | 130 | 142 | 109 | 158 | 109 | 34 |

ample of such a system. This is a reflection of the anomalously low bulk modulus since, as stated above, one can write, $C_{12} = B - \frac{2}{3}C'$. Table II shows that the tetragonal shear constant for UTe is not dramatically different from that of UC and US, whereas the bulk modulus is drastically different and the negative $C_{12}$ is caused by the very low $B$. In US the elastic constant $C_{12}$ is not negative, but this compound is clearly a borderline system since the measured value for $C_{12}$ is very low, $\sim$ 13 kbar. It is interesting to note that the calculated $C_{12}$ (deduced from Table II) for US is also low, $\sim$ 35 kbar, and actually in fairly good agreement with the experimental value. Thus, this indication of US being a borderline system, where the $5f$ states are on the boundary between being localized or delocalized, is quite well described by our LSDA calculations.

### B. Electronic structure

The calculated DOS of paramagnetic UC and ferromagnetic US are shown in Figs. 1 and 2, respectively. The total DOS is shown in Figs. 1(a) and 2(a), whereas the partial DOS is shown in Figs. 1(b) and 2(b). In agreement with previous calculations, the DOS for both systems is dominated by the $5f$ contribution. In UC the $5f$ band is split into a $5f_{5/2}$ and a $5f_{7/2}$ partial DOS, by about $\sim$ 0.1 Ry, due to the spin-orbit interaction. The C $2p$ DOS is centered $\sim$ 0.2 Ry below $E_F$ and overlaps with the U $5f$ states. It has previously been demonstrated that this leads to a substantial $p$-$f$ hybridization.[2] The value of the DOS at $E_F$ is 50 states/Ry and is higher than the value found in previous calculations.[2] This is due to

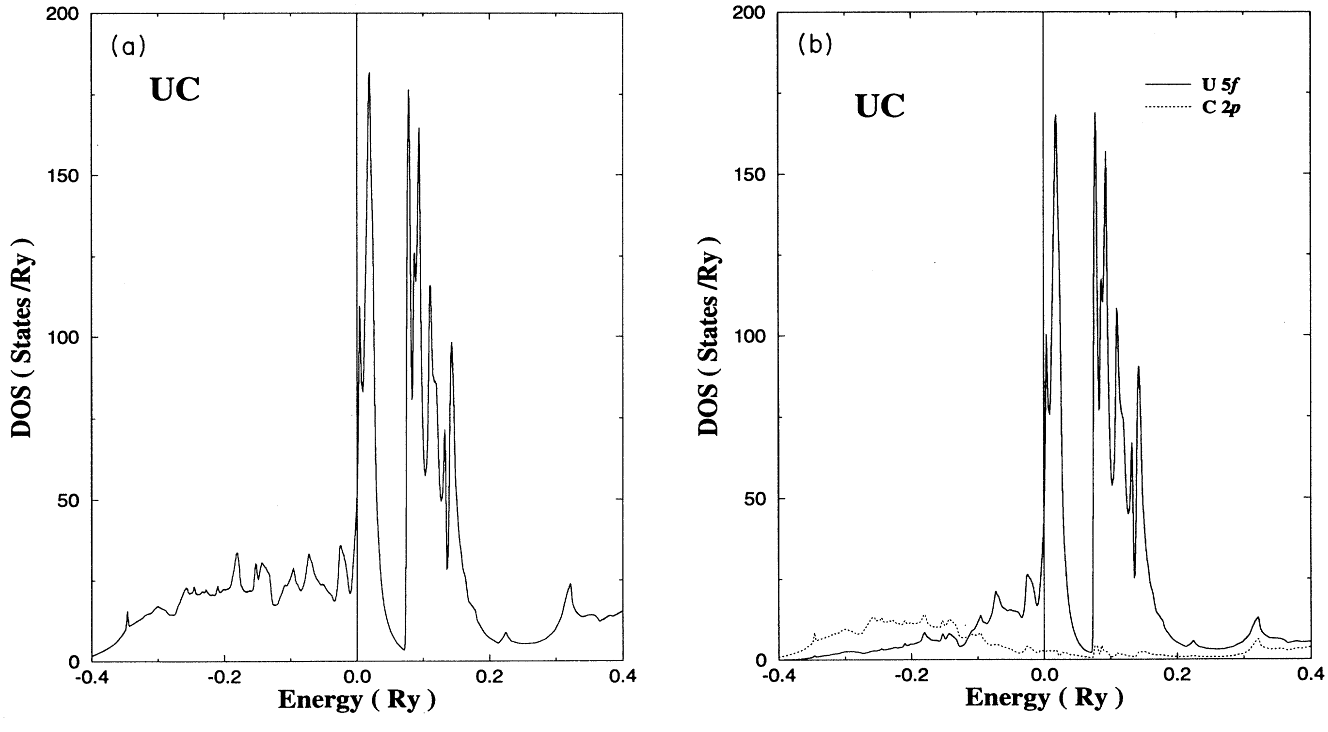

FIG. 1. Density of states (DOS) for UC. The total DOS is shown in (a) and the partial DOS of U $5f$ (solid line) and C $2p$ (dashed line) are shown in (b). Energies are in Ry and the Fermi level is at zero energy and is marked with a vertical line.

that in the present calculation the Fermi energy lies at the low energy side of the $5f_{5/2}$ peak, whereas previous theories calculate $E_F$ to be slightly lower in energy and thus the DOS at $E_F$ is lower. Nevertheless, in agreement with previous studies, we calculate the Stoner product to be less than one $[IN(E_F) = 0.9]$ and in agreement with experiment our calculations therefore, favor a paramagnetic ground state.

In US the $p$ bands do not overlap the $f$ states and correspondingly the $f$-$p$ hybridization is reduced compared to UC.[3] Furthermore, the $f$ states are exchange split by $\sim 0.1$ Ry. In this system the exchange splitting and spin-orbit interaction are of comparable magnitude. When comparing the bandwidths of UC and US, it is interesting to observe that they are quite comparable. Despite this fact UC appears more delocalized, since it is paramagnetic, whereas US has spin-polarized $5f$ states. Clearly the $5f$-band width is not the only parameter dictating the ground state properties. It is also interesting to observe that the values of the DOS at $E_F$ for UC and US are, in agreement with the measured $\gamma$ values, quite similar.

The energy band structures corresponding to the DOS presented in Figs. 1 and 2 are shown in Figs. 3 and 4, respectively. The energy bands of UC are in very good agreement with the results of Hasegawa and Yamagami,[4] whereas they differ somewhat from the energy band structure obtained by Brooks.[2] We note here that the differences observed in the electronic structure are not large enough to modify the calculated Fermi surface topology,[5] which was found to agree favorably with experiment.[6] For US, the energy band structure is more complicated to analyze since several bands cross the Fermi level. We observe also a few other features such that the $p$ bands, which are lying in the energy range $-0.55$ to $-0.25$ Ry, have a small exchange splitting, which is induced by the moment on the uranium site. The uranium $5f$ states are located around $E_F$ and as expected these bands are also exchange split.

### C. Charge density contours and chemical bonding

In Fig. 5, we show a projection of the charge density contour of UC on the [001] plane. The contours of US and UTe are not shown since they are quite similar to the contour of UC. In Fig. 5, we show the full charge density in (a) and the nonspherical density in (b). That is, in Fig. 5(b) we plot the density obtained when subtracting the spherically averaged density inside the muffin-tin spheres and the planar averaged density in the interstitial region. Note that this gives rise to a discontinuity of the density

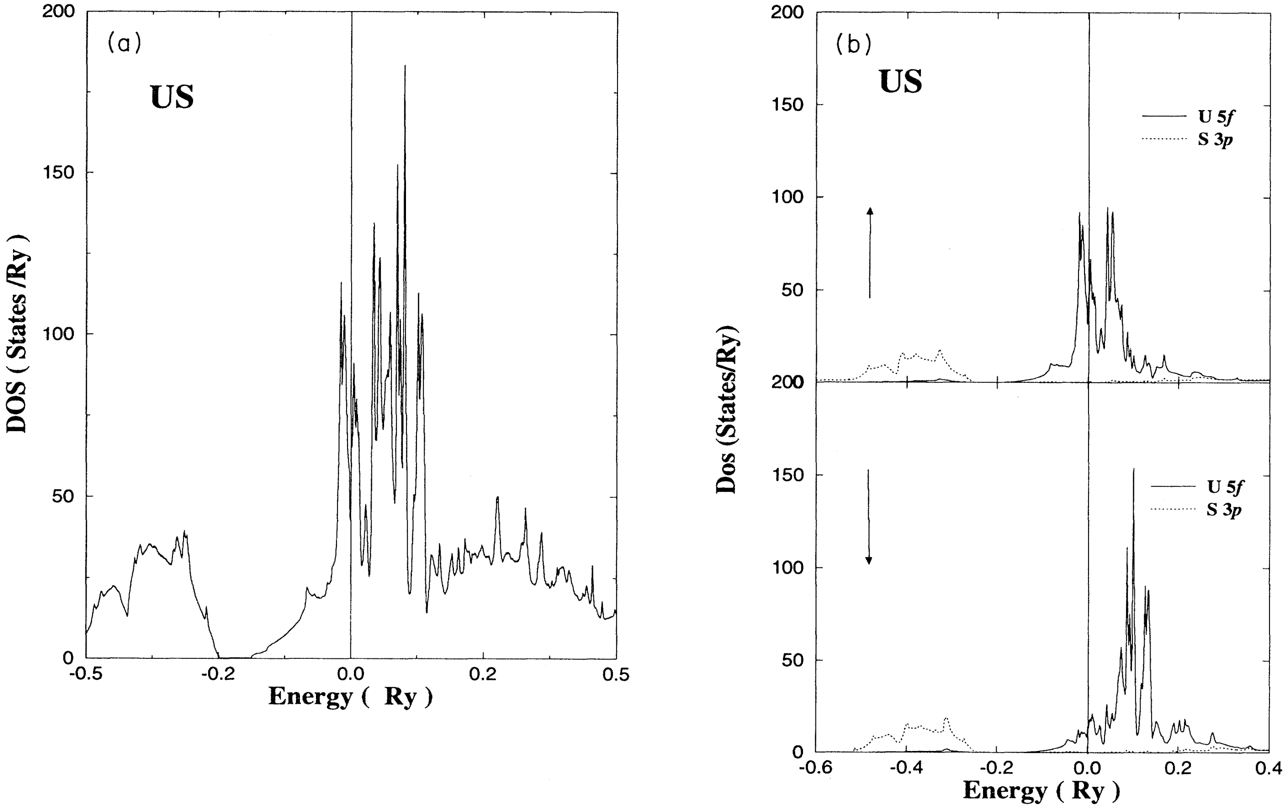

FIG. 2. Density of states (DOS) for US (from LSDA calculations). The total DOS is shown in (a) and the partial DOS of U $5f$ (solid line) and S $3p$ (dashed line) are shown in (b). The majority spin DOS is shown in the upper panel and minority spin DOS in the lower. Energies are in Ry and the Fermi level is at zero energy and is marked with a vertical line.

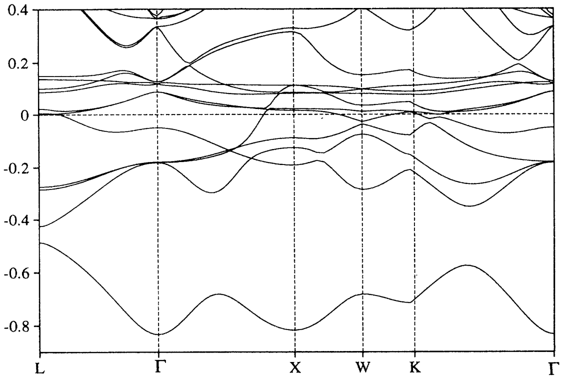

FIG. 3. Calculated energy bands for UC. Energies are in Ry and the Fermi level is marked by a horizontal dashed line.

in Fig. 5(b) since the spherically averaged density inside the muffin-tin spheres is not necessarily equal to the planar averaged density in the interstitial. In Fig. 5(a), i.e., for the full density, there is of course no discontinuity. The uranium atoms are located at the corners of the figure and there is also one uranium atom in the middle. The C atoms are located on the axis connecting the U atoms. Notice from this figure [especially Fig. 5(b)] that the charge density associated with the C atoms to a large degree is spherical, whereas the density around the U atoms has a larger degree of directionality. For instance, inside the uranium spheres the density shows lobes pointing in the direction to the nearest carbon atom. Thus, in agreement with the analysis of Brooks,[2,3] the chemical bonding in these compounds has a covalent contribution accompanying the metallic binding.

The calculated partial wave occupation numbers for UC, US, and UTe are shown in Table III. It should be pointed out here that these numbers are not unique, since to some extent they depend on the muffin-tin ($S_{m+}$) radii used in the calculations. In the present work, we have used the same ratio between the volume of the muffin-tin spheres and the unit cell volume, so that a comparison between the different compounds is meaningful (we list the muffin-tin radii used in Table III). Notice from Table III that the occupation numbers are quite different for the three systems. For instance, the $f$ occupation is close to 2 in UC, whereas it is $\sim$ 2.7 in UTe. For US, Reim and Schoenes[9] conclude that the $5f$ occupation is 2.9, which should be compared with our calculated value of 2.54. By adding the occupation numbers inside each muffin-tin sphere, we can extract information about the ionicity. For instance, there are 8.71, 8.91, and 9.00 valence electrons inside the cation muffin tins in UC, US, and UTe, respectively (remember that we are treating the $6p$ states as valence states). Moreover, there are 3.54, 5.91, and 5.53 valence electrons inside the anion muffin-tin spheres. The remaining charge is of course in the interstitial region. Thus, the cation has a charge of +3.29, +3.09, and +3.00, in UC, US, and UTe, respectively, and the anion has a charge of +0.46, +0.09, and +0.47, in UC, US, and UTe, respectively. Thus, the present results suggest that the cation gives up about three electrons to the interstitial region, whereas the anion gives up 0.0 – 0.5 electrons to the interstitial region.

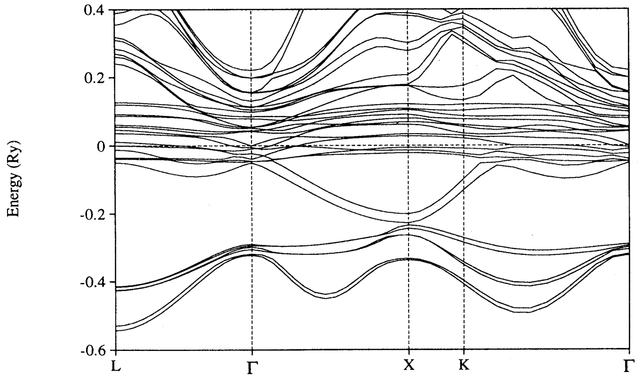

FIG. 4. Calculated energy bands for US (from LSDA calculations). Energies are in Ry and the Fermi level is marked by a horizontal dashed line.

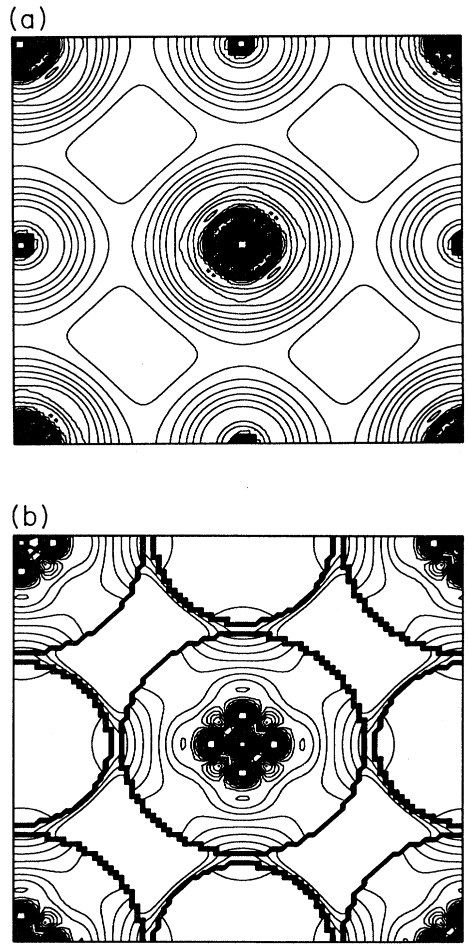

FIG. 5. (a) Calculated charge density of UC for a cut in the [001] plane. (b) Calculated charge density (nonspherical component) of UC for a cut in the [001] plane.

TABLE III. Calculated occupation numbers for UC, US, and UTe at the equilibrium volume.

| | Cation | | | | | Anion | | | |
|---|---|---|---|---|---|---|---|---|---|
| | $s$ | $p$ | $d$ | $f$ | $S_{mt}$ | $s$ | $p$ | $d$ | $S_{mt}$ |
| UC | 0.13 | 5.39 | 1.04 | 2.15 | 2.50 | 1.26 | 2.21 | 0.06 | 1.86 |
| US | 0.09 | 5.48 | 0.79 | 2.54 | 2.40 | 1.76 | 3.84 | 0.31 | 2.40 |
| UTe | 0.10 | 5.46 | 0.78 | 2.68 | 2.60 | 1.73 | 3.50 | 0.31 | 2.99 |

## IV. CONCLUSION

We have calculated the electronic structure, equilibrium volume, bulk modulus, and elastic constants of UC, US, and UTe, using a self-consistent full potential method, which is based on the local-spin-density approximation. The results for the bulk modulus are in overall agreement with previous calculations, which employed spherical potentials, and also in reasonable agreement with experiment — with the notable exception of UTe, where the calculated bulk modulus is a factor of 3 too large. We have also performed calculations for US using the LSDA+OP formalism and found acceptable agreement with experimental magnetic data. As regards the chemical bonding, the OP correction has little effect on US and the calculated equilibrium volume, $C'$, and $B$ are very similar for the LSDA and LSDA+OP formalisms.

The calculated elastic constants are also in agreement with published measurements for UC and US and evidence suggests that the electronic structure of these two compounds is described quite well by the local density approximation. The calculated tetragonal shear constant, $C'$, is about 80% larger than measurements for UTe and the calculated bulk modulus is a factor of 3 larger than the experimental value. The measured, anomalously low, bulk modulus of UTe leads to a negative Poisson's ratio, which is not reproduced by our calculations. This is an obvious failure, which we ascribe to errors in the local density approximation and this leads us to suspect that UTe is a dense Kondo or mixed valence compound.

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