Structural behavior of α-uranium with pressures to 100 GPa

T. Le Bihan,[1] S. Heathman,[2] M. Idiri,[2] G. H. Lander,[2,3] J. M. Wills,[3] A. C. Lawson,[3] and A. Lindbaum[4]
[1]*European Synchrotron Radiation Facility, Boite Postale 220, F-38043 Grenoble Cedex, France*
[2]*European Commission, JRC, Institute for Transuranium Elements, Postfach 2340, D-76125 Karlsruhe, Germany*
[3]*Los Alamos National Laboratory, Los Alamos, New Mexico 87545*
[4]*Institute for Solid State Physics, Vienna University of Technology, Wiedner Hauptstrasse 8-10/138, A-1040 Wien, Austria*
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The structural behavior of α-uranium at room temperature has been studied up to 100 GPa in diamond anvil cells using angle-dispersive x-ray diffraction at a synchrotron source. The orthorhombic *Cmcm* structure is stable to at least 100 GPa. We present details of the variation of all structural parameters, derived from Rietveld analysis of the diffraction patterns: the lattice parameters *a*, *b*, and *c*, and the positional parameter *y*, as a function of pressure. Precise data, as well as the use of different media for the pressure transmission, allow us to question previous values of several parameters deduced by x-ray diffraction, especially the bulk modulus, and we obtain a revised bulk modulus of $B_0 = 104(2)$ GPa with $B_0' = 6.2(2)$. We have also performed accurate (zero-temperature) electronic structure calculations with full structural relaxation up to 100 GPa to test theory against our experimental results. The magnitude and trends of the calculated structural parameters are in reasonable agreement with experiment. In contrast, our bulk modulus calculated at our zero-pressure volume is $B_0 = 136$ GPa and $B_0' = 5.07$, in agreement with previous calculations, differing markedly from experimental values.

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I. INTRODUCTION

The behavior of actinide metals under pressure can be differentiated into two groups. The $5f$ electrons in the elements Th–Pu show itinerant behavior and contribute to the bonding, whereas in the following elements including Am and beyond the $5f$ states are localized and nonbonding.[1] A study of these materials as a function of pressure thus yields important information about the role of the $5f$ electrons in the solid. A good example is our recent study of Am (Ref. 2) and Am-Cm alloy (Ref. 3), which provide new information about the involvement of the $5f$ electrons in the metallic bonding in Am. We determined also that the fourth high-pressure phase of Am, which was thought to have the α-uranium crystal structure *Cmcm*, has in fact a primitive orthorhombic *Pnma* structure. These two structures are closely related. In view of this, we decided to perform high-pressure experiments on uranium under the same conditions to determine if the structure remained *Cmcm* at all pressures up to 100 GPa.

Below the formation of the β phase at 935 K, uranium crystallizes in the α phase with the orthorhombic space group *Cmcm* (no. 63), with uranium atoms at Wyckoff positions 4(c): $(0, \pm y, \pm \frac{1}{4})$ with $y = 0.1024$ at room temperature.[4] Many articles about the structural behavior of α-uranium under pressure at ambient temperature have been published,[5–11] none of which reports results of experiments using the angle-dispersive technique with diamond anvil cells (DAC). As we have shown,[2] this technique, combined with Rietveld analysis of diffraction patterns, provides more information than the older methods. We find that α-U does indeed remain in the *Cmcm* phase up to 100 GPa. In addition, the quality of our data has allowed us to determine that the bulk modulus is considerably lower than previously determined by x-ray techniques. We report also a first-principles theoretical investigation of the parameters in α-U as a function of pressure. For the most part there is reasonable agreement between theory and experiment, except for the bulk modulus, and in details of the compressibility of the individual axes.

II. EXPERIMENTAL DETAILS

Small pieces of depleted uranium were handled under argon atmosphere in a glovebox at the Institute for Transuranium Elements. Samples were loaded into three different DAC types: one of Syassen-Holzapfel type [opening angle: 14° (2θ)] with diamond flats of 400 μm, one of Le Toullec type [opening angle: 24° (2θ)] with beveled 300-μm diamonds, and the other of Cornell type [opening angle: 21° (2θ)] with beveled 200-μm diamonds, together with pressure-transmitting medium (liquid N_2 or silicone oil) and pressure gauge (ruby crystal or Pt powder).

As a platinum pressure marker was used to estimate the pressure, we performed an experiment to verify the equation of state parameters of Pt. A loading was made with ruby as pressure gauge and we found, for $V_0 = 60.4012$ Å^3, $B_0 = 282.8 \pm 5.0$ GPa and $B_0' = 5.74 \pm 0.30$, in agreement with the values published by Holmes *et al.*[12] The pressures measured by using ruby and platinum in the uranium experiments were in good agreement. Nevertheless, in order to check if our Pt equation of state parameters described well our experimental conditions at high pressure, we took one image with Cu as pressure calibrant.[13] We obtained, at 79 GPa, a perfect agreement between the two metal gauges.

The experiments were performed at the European Synchrotron Radiation Facility (ESRF) on the ID30 undulator beam line in an angle-dispersive mode using monochromatic radiation. A channel-cut, water-cooled Si(111) monochromator was used to produce a monochromatic beam of either

33.17 keV (0.3738 Å) or 61.33 keV (0.2021 Å).

In the case of the experiment with the Syassen-Holzapfel type DAC ($\lambda = 0.2021$ Å) the beam was collimated to 90 $\times 90$ μm^2, whereas for the other experiments the beam was focused with vertical and horizontal Kirkpatrick-Baez mirrors to full widths at half maximum close to 10 μm. Two-dimensional images were recorded on a MAR345 image plate detector or on a Bruker charge-coupled device (CCD) camera. The Debye-Scherrer patterns showed that there was no preferred orientation and that a large number of grains were sampled. The fully integrated profiles, obtained with the European Synchrotron Radiation Facility FIT2D software, were refined using the Rietveld method with the FULLPROF program.[14]

Theoretical calculations were performed using a full-potential electronic structure method that uses muffin-tin orbitals for basis states (FPLMTO).[15] Exchange and correlation were treated in the generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof.[16] Denoting basis states by $t(nl)$, where t is the number of kinetic energies and n and l the principal and orbital parameters, our basis was $2(6s6p)3(7s7p)2(6d5f)$, resulting in 88 basis states per U atom. Calculations were fully relativistic; muffin-tin radii were kept fixed to avoid any ambiguity in equilibrium volume.[17] Structural relaxation was accomplished using a simple conjugate gradient scheme to minimize the energy with respect to the orthorhombic lattice parameters a, b, and c and the structural parameter y, with the volume imposed as a constraint. Integrals over the Brillouin zone were performed by linear interpolation on tetrahedra with an energy correction[18] using 234 irreducible points in the Brillouin zone. Using this set, the calculated values were converged to $<1\%$.

III. RESULTS

Initial experiments were performed using the Syassen-Holzapfel type DAC. For the first run, silicone oil was used as the pressure-transmitting medium and experiments were carried out to a pressure of 10.5 GPa. This was followed by a second run under identical conditions except that nitrogen was loaded as the pressure medium. For this second run, the sample was measured up to 47(2) GPa in 20 steps of increasing pressure. A second loading under identical experimental conditions was then made at atmospheric pressure to obtain precise initial lattice parameters and volume of the unit cell.

A third experimental run was performed with the Le Toullec type DAC. As for the preceding run, we first took one image at atmospheric pressure, and then, with another loading, we reached 67(3) GPa in 20 steps. This time, we put more sample in the gasket hole to check if a poorer hydrostatic condition could influence the structural behavior of uranium.

To obtain high-pressure data up to 100 GPa, we performed a run using a Cornell type diamond anvil cell and collected a further 23 images from atmospheric pressure to 100(5) GPa. As explained above, a final run was conducted to take a single image with Cu as pressure gauge.

The initial lattice parameters were determined as $a = 2.8553(1)$ Å, $b = 5.8701(2)$ Å, $c = 4.9568(2)$ Å, $V = 83.081(6)$ Å^3, in excellent agreement with the literature.[19] No UO_2 lines indicating oxidation of the sample were observed in these runs. Our calculated lattice parameters are $a = 2.831$ Å, $b = 5.797$ Å, and $c = 4.957$ Å, at the theoretical equilibrium; at the experimental volume, the values are $a = 2.852$ Å, $b = 5.841$ Å, and $c = 4.982$ Å. Our calculated structural parameter is $y = 0.1020$ at both volumes. These values are in good agreement with experiment. Söderlind[20] recently calculated structural parameters at ambient pressure and obtained similar values.

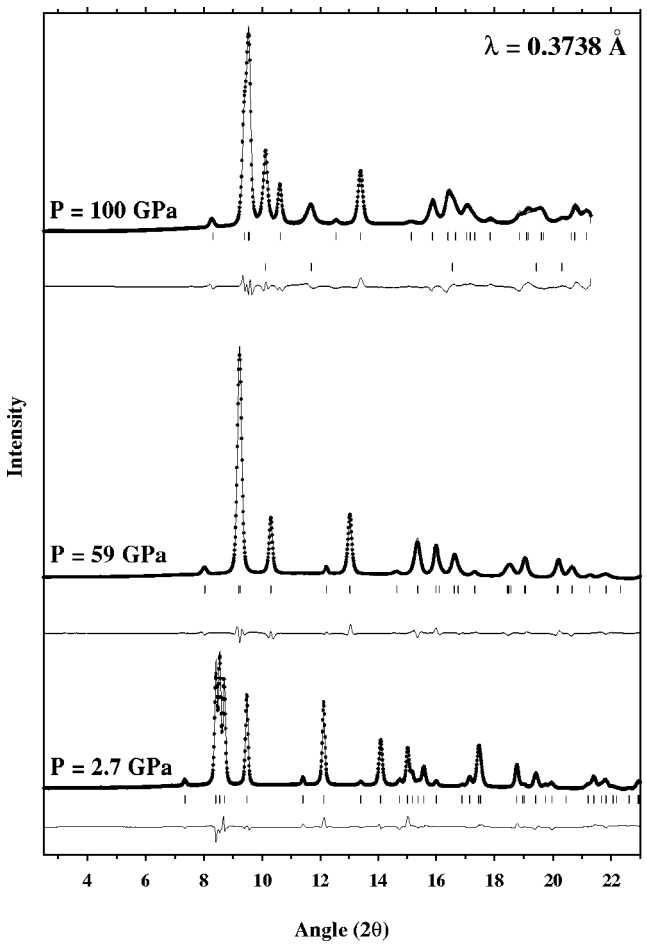

FIG. 1. Experimental data (points) together with Rietveld profile fits of the synchrotron data at the listed pressures. The tick marks show the position of the reflections and the thinner lines below the main profile are the difference profiles. The reliability factor R_{Bragg} is 7.83% at 2.7 GPa, 3.78% at 59 GPa, and 6.70% at 100 GPa. The second phase in the pattern at 100 GPa is the Pt pressure marker.

Figure 1 shows angularly averaged powder-diffraction patterns fitted with the Rietveld analysis for three different pressures. No phase change was observed up to 100 GPa, the maximum pressure reported.

In Fig. 2(a) the results of our experimental determination of the fractional volume are shown. As we shall discuss later, it is clear that *some* of the data on this plot are not consistent with a smooth variation of V/V_0. We focus on the data taken as "N_2 hydrostatic+ruby." With these data we have fit the Birch-Murnaghan equation of state:[21]

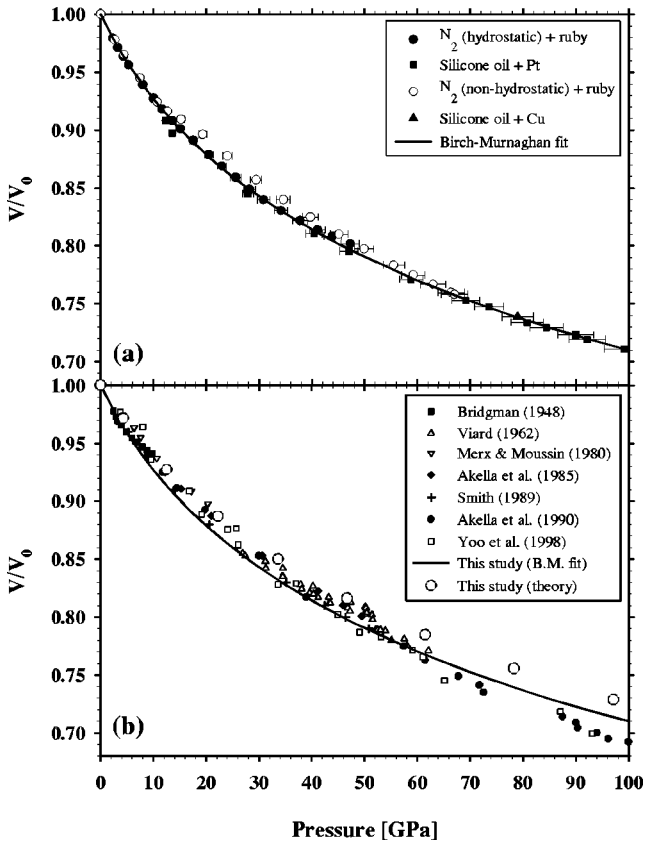

FIG. 2. Relative volume as a function of pressures for α-U. (a) All data taken in the present series of experiments. The Birch-Murnaghan fit to the ''best data'' (see text) is shown as the solid line. It gives a bulk modulus $B_0=104(2)$ GPa and $B_0'=6.2(2)$. (b) The Birch Murnaghan fit is again shown as a solid line. The data points are from all previous studies of α-U. The additional references are Bridgman (1948) discussed and revised in Gschniedner (1964) (Ref. 22), Viard (1962) (Ref. 23), Merx and Moussin (1980) (Ref. 5), Akella, Smith, and Weed (1985) (Ref. 6), Smith (1989) (Ref. 24), Akella *et al.* (1990) (Ref. 8), and Yoo, Cynn, and Söderland (1998) (Ref. 11).

$$P=\tfrac{3}{2}B_0\left[\left(\frac{V}{V_0}\right)^{-7/3}-\left(\frac{V}{V_0}\right)^{-5/3}\right]\times\left\{1-\tfrac{3}{4}(4-B_0')\left[\left(\frac{V}{V_0}\right)^{-2/3}-1\right]\right\}$$

to the experimental points. The values obtained were $B_0=104(2)$ GPa and $B_0'=6.2(2)$.

In the Fig. 2(b) we reproduce the Birch-Murnaghan fit to our ''best'' data, together with the experimental points from some of the earlier studies.[22–24] It is apparent that the earlier data lie predominantly *above* the solid curve, and hence will give a B_0 significantly *greater* than the value we obtain.

To emphasize this point, we compare the pressure-volume curves up to 12 GPa taken with silicone-oil- and nitrogen-pressure-transmitting mediums in Fig. 3. This shows a marked discontinuity starting at around 4–5 GPa for the oil loading. This anomaly has been observed previously in our work on the UX_3 compounds[25] and by other authors, and is

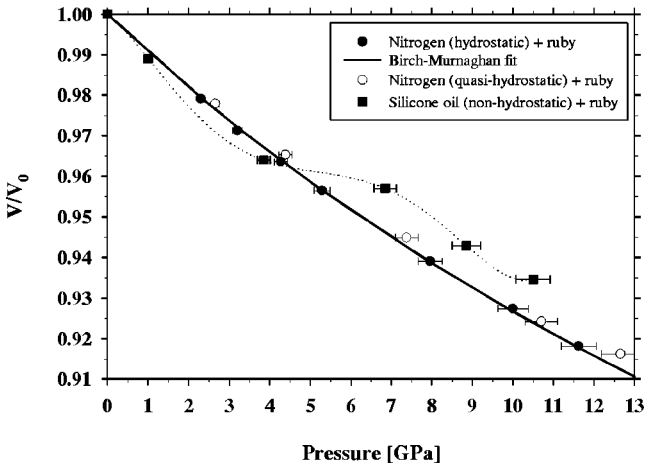

FIG. 3. Relative volume as a function of pressures for α-U in the low-pressure region, showing the effect of pressure-transmitting medium.

now fairly conclusively thought to be due to the freezing of the pressure medium and consequent work hardening.[26–28] The effect on the relative volume and lattice parameters of uranium is particularly evident with our high-resolution synchrotron data and may explain why many earlier measurements overestimated the compressibility. We also show the calculated pressure volume curve.

Figure 4 shows the relative changes in the lattice parameters as a function of reduced volume along with calculated parameters. The slowest changing axis (least compressible) is c, and theory reproduces this effect. Experiment finds that the a axis is most compressible up to 100 GPa. At low pressures (and zero temperature), theory predicts that a and b have similar compressibilities. At approximately 25 GPa, theory has b/b_0 crossing a/a_0 and becoming the more compressible axis. Parameters calculated using a thermal population decrease the difference between theory and experiment in this regard (see the discussion in the summary below), but

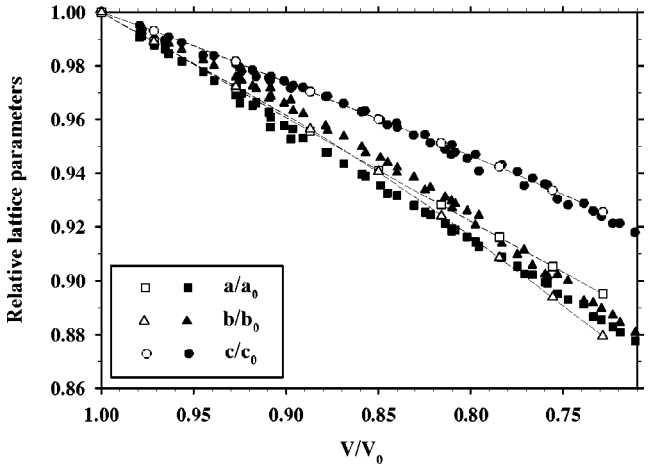

FIG. 4. Relative lattice parameters as a function of relative volume. The experimental values are given as filled symbols (circles for c/c_0, squares for a/a_0, and up triangles for b/b_0) and the theory as open symbols with a polynomial fit through them of the dashed lines.

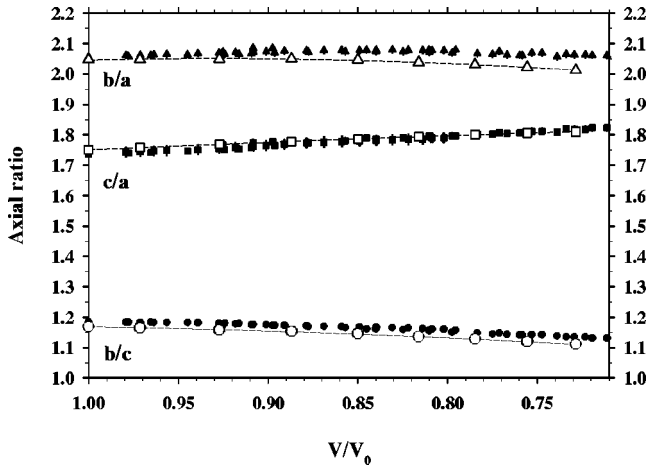

FIG. 5. Axial ratios as a function of relative volume. The solid symbols are experiment. The open symbols joined with dashed lines are the theory.

not significantly. Figure 5 shows the axial ratios again as a function of reduced volume. The scale in this plot is quite large, in order to show all three ratios, but it does show that in general, theory is able to reproduce the effects of pressure in α-U quite well.

One unusual aspect of the fractional change of the lattice parameters with pressure is the fact that at intermediate pressures the a/a_0 and b/b_0 curves (Fig. 4) diverge quite considerably, and then tend to merge again at higher pressure. This is a consequence of the elastic anisotropy of α-U. Figure 6 shows the experimental consequences of this in a more direct way by showing the positions of three of the first diffraction lines for three different pressures. Although there is significant line broadening at 100 GPa (this is a phenomenon almost always observed in high-pressure x-ray experiments), there is a tendency with increasing pressure for the first three diffraction lines to be at almost the same *d* space (at 59 GPa) and then to separate again (at 100 GPa), as they were at ambient pressure.

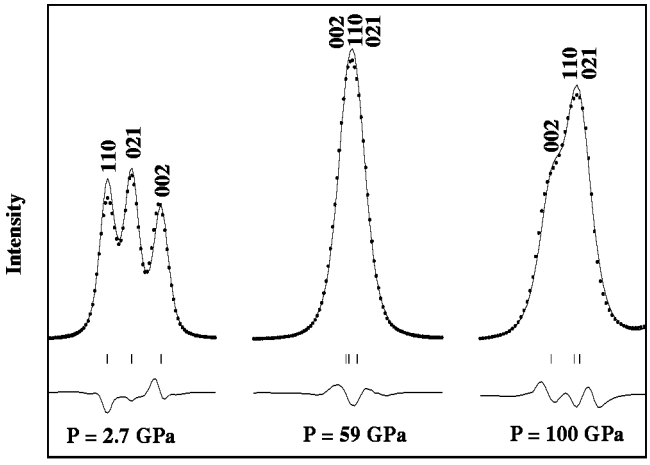

FIG. 6. Behavior of the positions of the long *d*-spacing reflections (110), (021), and (002) at three different pressures. This shows, as in Fig. 1, that the positions of the peaks can be accurately determined by the fitting procedure.

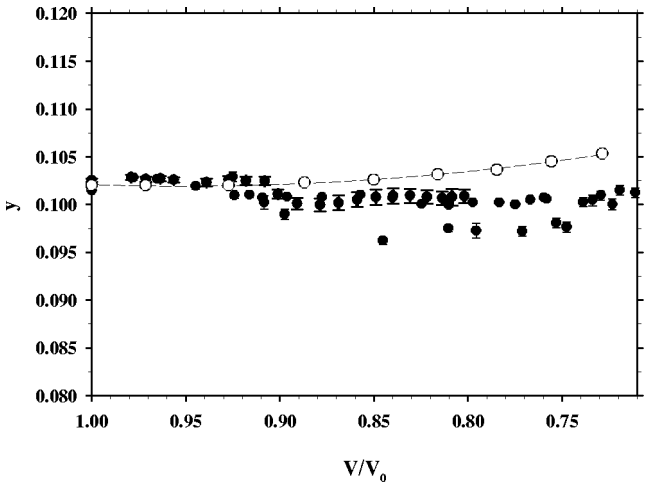

FIG. 7. Atomic positional parameter *y* of the α-U (*Cmcm*) structure as a function of relative volume. The theory values are shown as open points. The experimental values below 0.100 are probably due to a poor Rietveld fit.

Finally, in Fig. 7 we show the variation of the positional parameter as a function of reduced volume. This is the hardest parameter to refine, as it depends on the *intensities* of the diffraction lines rather than their *position*. We notice that the theory is in reasonable agreement at low pressures but predicts a slightly greater variation than is observed experimentally, especially at high pressure.

IV. DISCUSSION

The most important results of our work are that (a) we have confirmed that the α-U structure (*Cmcm*) is stable to 100 GPa and (b) the bulk modulus is lower than all previous determinations with *x rays*. With respect to the first point, α-U is exceptional in the sense that it is the only actinide that does not exhibit any phase transition below 100 GPa. This fact is in agreement with previous theory,[10] as well as our current efforts. Calculations of Pénicaud[29] predict a transition for $\sim$31% compression of α-U; at 100(5) GPa, we obtain a compression equal to 29%.

The bulk modulus determined experimentally in this study 104(2) GPa [$B_0'=6.2(2)$] is much lower than that deduced from previous x-ray experiments where B_0 and B_0' are respectively, 143.4 GPa and 3.76 (Ref. 5), 125 GPa and 6.2 (Ref. 6), 147(3) GPa and 2.8(3) (Ref. 7), 138.7 GPa and 3.78 (Ref. 8), 135.5 GPa and 3.79 (Ref. 11). We have argued in our presentation of the results that we believe the previous x-ray measurements are in error and do not completely account for the effect of freezing of the pressure medium (see Figs. 2 and 3) and that this has led to a systematical overestimate of B_0. It is the low-pressure part of the equation-of-state relationship (Fig. 2) that is particularly important in determining B_0 and, as shown in Fig. 3, this is the region that is strongly influenced by nonhydrostatic conditions. Moreover, in many cases the number of data points in previous work is small compared to ours (see especially Ref. 11) and this has exacerbated the difficulty in deducing B_0. Clearly, the quality of data obtained in the present experiments, once

TABLE I. Values of the bulk modulus as derived from various measurements in the literature. Note that some of the early work, quoted in Fisher and McSkimin (Ref. 30) had problems with obtaining a random grain orientation in α-U. For this reason they are not quoted, although they generally lie in the region of 90–120 GPa. Error bars are not given in many measurements, but probably are of the order of 2–4 %.

Type of measurement	B_0 (GPa)	Effective temp. (K)	Reference
Mechanical displacement	101	300	Gschneidner, 1964[a] (Ref. 22)
Ultrasonic	111	300	Fisher and McSkimin 1958 (Ref. 30)
Early specific heat	~55–80	$T\rightarrow 0$ K	See Ref. 4
High-P x rays	143	300	Merx and Moussin 1980 (Ref. 5)
High-P x rays	125	300	Akella, Smith, and Weed 1985 (Ref. 6)
High-P x rays	147	300	Dabos *et al.*, 1987 (Ref. 7)
High-P x rays	139	300	Akella *et al.*, 1990 (Ref. 8)
High-P x rays	136	300	Yoo, Cynn, and Söderland 1998 (Ref. 11)
Ultrasonic	114	300	Yamanaka *et al.*, 1998 (Ref. 31)
Neutron-diffr. T factors	112	300	Lawson *et al.*, 2000 (Ref. 32)
Specific heat	107(1)	$T\rightarrow 0$ K	Lashley *et al.*, 2001 (Ref. 33)
High-P x rays	104(2)	300	Present work

[a]Values of Bridgman (1948) reevaluated by Gschneidner (Ref. 22).

true hydrostatic conditions are obtained, provides a great improvement in accuracy of measured bulk modulus. This is in a large part due to the use of the high brilliance of the third generation synchrotron source and the use of the angular dispersive technique.

It is then instructive to return to other methods of measuring B_0. Many measurements probe indirectly the lattice compressibility. The most common is the relation between B_0 and θ_D, the Debye temperature, which is given by

$$\theta_D = \frac{h}{2\pi k_B}\left(\frac{6\pi^2}{\Omega}\right)^{1/3}\sqrt{\frac{B_0 N_0 \Omega}{M}},$$

where Ω is the atomic volume ($=20.74$ Å^3), N_0 is Avogadro's number, and M is the mass of the atoms ($=238$ amu). There are a number of methods of determining θ_D and we have listed some of the derived B_0 values, together with the B_0's derived from x-ray work in Table I.[30–33] The estimated difference between the isothermal and adiabatic bulk moduli is about 3%, and we have neglected it here.

Table I, in which the entries are in chronological order, shows interesting trends. Initially, the early measurements gave $B_0 \sim 105$ GPa. It is worth highlighting the pioneering experiments of Fisher and McSkimin on single crystals in this series of experiments. However, the early specific-heat experiments clearly deduced incorrect values for θ_D, probably because of effects of intergranular stresses.[34] By the mid-1970s, however, the x-ray technique was thought superior and a number of experiments gave values *higher* than those reported earlier.

The bulk modulus was then accepted as ~140 GPa, and this was reinforced when theory also obtained a similar value. However, it is now clear that these higher experimental values are incorrect, for the reasons discussed in this paper. In the last three years, three *independent* investigations have arrived at a bulk modulus that is essentially unchanged from that determined by Bridgman 50 years ago.

The great difficulty that this now poses is that the latest theories, including the one we report, obtain a significantly higher value for the B_0. Our calculations give 136 GPa. Pénicaud[29] obtains 147.5 GPa and Söderlind[20] obtains 130 GPa. Although earlier calculations using the atomic sphere approximation and a hypothetical crystal structure (fcc), such as those by Skriver, Andersen, and Johansson[35] and Pénicaud[36] were lower at 115 and 117 GPa, respectively, the more recent calculations have all tended to be about 140 GPa. These are then in disagreement with the experiment.

The orthorhombic structure of α-U is fairly complex; nevertheless, the calculations we report, with complete structural relaxation, provide a good test of theory. The theoretical calculations are performed at zero temperature, whereas the experiment is performed at room temperature. In normal materials, the largest effect of temperature is thermal expansion; this is an unlikely source for the discrepancy we report. We note that the difference in equilibrium volume at 100 GPa between the experiment (with $B_0=104$ GPa) and theory (with $B_0=136$ GPa) is only 2.1%, and the bulk modulus calculated at the experimental volume is 124 GPa, decreased by 9%. We have investigated thermal effects on the calculated structural parameters by performing structural relaxation using a thermal population of Kohn-Sham eigenstates corresponding to a temperature of ~1000 K. There is no significant change in the bulk modulus. Interestingly, the pressure dependence of the lattice parameters a and b is changed so that b changes more slowly than a at low pressure, which is in better qualitative agreement with our experimental results than the zero-temperature results. On increasing pressure, however, b again increases more rapidly than a; b/b_0 crosses a/a_0 at approximately 40 GPa. We find this result interesting, but hardly conclusive.

Uranium has additional complexity in that this material is subject to charge density wave (CDW) instabilities at low temperatures.[4] This instability is also present in our electronic structure calculations. Calculations have demonstrated that the highest-temperature CDW, which occurs at 43 K, is the result of a Fermi-surface instability quantitatively described by electronic structure theory.[37] This instability may affect the connection between zero-temperature calculation and room-temperature experiment.

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[1] *Los Alamos Science, Challenges in Plutonium Science*, edited by N. G. Cooper, No. 26, Vol. I (2000).
[2] S. Heathman, R. G. Haire, T. Le Bihan, A. Lindbaum, K. Litfin, Y. Méresse, and H. Libotte, Phys. Rev. Lett. **85**, 2961 (2000); A. Lindbaum *et al.*, Phys. Rev. B **63**, 214101 (2001).
[3] T. Le Bihan, R. G. Haire, S. Heathman, M. Idiri, and A. Lindbaum, J. Nucl. Sci. Technol. **3**, 45 (2002).
[4] G. H. Lander, E. S. Fisher, and S. D. Bader, Adv. Phys. **43**, 1 (1994).
[5] H. Merx and C. Moussin, in *High Pressure Science and Technology*, edited by B. Vodar and Ph. Marteau (Pergamon, Paris, 1980), Vol. 1, p. 204.
[6] J. Akella, G. S. Smith, and H. Weed, J. Phys. Chem. Solids **46**, 399 (1985).
[7] S. Dabos, C. Dufour, U. Benedict, and M. Pagès, J. Magn. Magn. Mater. **63–64**, 661 (1987).
[8] J. Akella, G. S. Smith, R. Grover, Y. Wu, and S. Martin, High Press. Res. **2**, 295 (1990).
[9] J. Akella, S. Weir, and G. S. Smith, LLNL Research Monograph (1993).
[10] J. Akella, S. Weir, J. M. Wills, and P. Söderlind, J. Phys.: Condens. Matter **9**, L549 (1997).
[11] C. S. Yoo, H. Cynn, and P. Söderlind, Phys. Rev. B **57**, 10 359 (1998).
[12] N. C. Holmes, J. A. Moriarty, G. R. Gathers, and W. J. Nellis, J. Appl. Phys. **66**, 2962 (1989).
[13] W. J. Carter, S. P. Marsh, J. N. Fritz, and R. G. McQueen, *Accurate Characterization of the High-Pressure Environment*, NBS Special Publication No. 326, edited by E. C. Lloyd (U.S. Government Printing Office, Washington, D.C., 1971), p. 147.
[14] J. Rodríguez-Carvajal, Physica B **192**, 55 (1993).
[15] J. M. Wills and O. Eriksson, Phys. Rev. B **45**, 13 879 (1992).
[16] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. **77**, 3865 (1996).
[17] L. Nordström, J. M. Wills, P. H. Andersson, P. Söderlind, and O. Eriksson, Phys. Rev. B **63**, 035103 (2001).
[18] P. E. Blöchl, O. Jepsen, and O. K. Andersen, Phys. Rev. B **49**, 16 223 (1994).
[19] C. S. Barrett, M. H. Mueller, and R. L. Hitterman, Phys. Rev. **129**, 625 (1963).
[20] P. Söderlind, Phys. Rev. B **66**, 085113 (2002).
[21] F. Birch, Phys. Rev. **71**, 809 (1947).
[22] K. A. Gschneidner in *Solid State Physics*, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1964), Vol. 16, p. 275.
[23] J. Viard, in *Les Ondes de Détonation* (CNRS, Paris, 1962), p. 383.
[24] G. S. Smith, Phys. Lett. A **140**, 431 (1989).
[25] T. Le Bihan, S. Heathman, S. Darracq, C. Abraham, J. M. Winand, U. Benedict, High Temp.-High Press. **27-28**, 157 (1995–1996).
[26] J. W. Otto, J. K. Vassiliou, and G. Frommeyer, High Press. Res. **17**, 13 (2000).
[27] J. W. Otto, J. K. Vassiliou, and G. Frommeyer, Phys. Rev. B **57**, 3253 (1997).
[28] J. W. Otto, J. Appl. Crystallogr. **30**, 1008 (1997).
[29] M. Pénicaud, J. Phys.: Condens. Matter **14**, 3575 (2002).
[30] E. S. Fisher and H. J. McSkimin, J. Appl. Phys. **29**, 1473 (1958); this work is also summarized in Ref. 4.
[31] S. Yamanaka, K. Yamada, T. Tsuzuki, T. Iguchi, M. Katsura, Y. Hoshino, and W. Saiki, J. Alloys Compd. **271-273**, 549 (1998).
[32] A. C. Lawson, B. Martinez, J. A. Roberts, B. I. Bennett, and J. W. Richardson, Philos. Mag. B **80**, 53 (2000).
[33] J. C. Lashley, B. E. Lang, J. Boerio-Goates, B. F. Woodfield, G. M. Schmiedeshoff, E. C. Gay, C. C. McPheeters, D. J. Thoma, W. L. Hults, J. C. Cooley, R. J. Hanrahan, and J. L. Smith, Phys. Rev. B **63**, 224510 (2001).
[34] J. Lashley (private communication).
[35] H. L. Skriver, O. K. Andersen, and B. Johansson, Phys. Rev. Lett. **41**, 42 (1978).
[36] M. Pénicaud, in *Shock Waves in Condensed Matter*, edited by J. R. Asay, R. A. Graham, and G. K. Straub (North Holland, Amsterdam, 1983), p. 61.
[37] L. Fast, O. Eriksson, B. Johansson, J. M. Wills, G. Straub, H. Roeder, and L. Nordström, Phys. Rev. Lett. **81**, 2978 (1998).