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Structure, formation energies and elastic constants of uranium metal investigated by first principles calculations

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ABSTRACT

The structures, formation energies and elastic constants of α-U, β-U, γ-U, fcc-U, hcp-U and bct-U were investigated by first principles calculations. It turns out that the structures described by the space groups no. 118 and 136 can be identical for the β-U and that the symmetry of β-U should belong to the space group no. 136. Interestingly, it is also shown that β-U might exhibit some isotropic behaviors and that both γ-U and fcc-U are unstable in the ground state because their Zener's shear constants are negative. The results and conclusion obtained in present study are supported by or consistent with others theoretical prediction and experimental observations.

1. Introduction

The actinides uranium has received a lot of attention for its nuclear properties and the application in the field of nuclear energy. At one atmospheric pressure, uranium metal exhibits three allotropes, i.e. α-U, β-U and γ-U, upon heating from the low temperature to the melting point [1]. The low temperature phase α-U, stably existing up to 669 °C, is face-centered orthorhombic (fco, space group no. 63, Cmcm) and there are four atoms per unit cell. The high temperature phase γ-U, stably existing from 776 °C to the melting point of 1135 °C, is body-centered cubic (bcc, space group no. 229, Im3m) and there are two atoms per unit cell. The β-U stably exists in a small temperature range 669–776 °C [1]. The structures of α-U and γ-U have been well established for a long time. For the structure of β-U, however only one fact is accepted that it is tetragonal and there are 30 atoms per unit cell. Concerning the exact arrangement of the 30 atoms in the unit cell, there are more than usual number of contradictions and uncertainties. In this regard, Donohue has presented a thorough survey of the controversies [2].

The structures, formation energies and elastic constants are the basic physical properties of a material. To experimentally determine these properties of uranium metal is intrinsically complicated by its' high reactivity and radioactivity. Alternatively, these properties can also be acquired by some theoretical approaches such as first principles calculations. In recent decades, the first principles calculations were therefore frequently employed to facilitate the investigation on the structure and properties of α-U. For example, Boettger et al. successfully calculated the atomic volumes, bulk modules, and relative stabilities of the fcc-U, bcc-U, and α-U [3]. These structural properties and bulk modulus of α-U were also be investigated by Söderlind with first principles calculations [4]. It turns out that the calculated results compared very favorably with experimental observations. Besides, based on the ab initio derived dynamical matrices, Bouchet investigated the vibrating behaviors of α-U at low temperature [5].

In present study, we intend to investigate the structural and elastic properties of uranium metal by using first principles calculations. Especially, we pay the main attention to the structure of β-U by considering the facts below. In order to obtain the single crystal of β-U at room temperature, 1.4 at.% Cr was usually added as the stabilizer in experiments [6–9]. However, it is not known whether these alloys have the same structure and property as the pure β-U. In addition, to the authors' knowledge, there were few first principles studies on β-U reported previously. The present work is therefore dedicated to studying the structure and elastic constants of β-U by using first principles calculations. The present work would also provide a basis for future investigating the effect of impurities and lattice defects on the properties of uranium metal. For example, based the calculated results, an *n*-body potential has been developed and applied to simulate the structural transformation and diffusion behavior of uranium metal upon dissolving other metal atoms [10].

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2. Method and procedure of first principles calculations

In present study, the first principles computations of the mechanical and structural properties were carried out by using the first principles simulation package of CASTEP (Version 5.5) [11]. Theoretically, because of the open crystalline structure, uranium metal is best treated with the full potential methods [12,13]. The PAW functions for uranium supplied with CASTEP, PW91 exchange-correlation functional and the generalized gradient approximation (GGA) were adopted without modification [14–18]. The crystalline structures were first optimized by using the BFGS method [19] and then the elastic constants and bulk modules were calculated. The implementation of BFGS scheme in CASTEP involves a Hessian matrix in the mixed space of internal and cell degrees of freedom, so that both lattice parameters and atomic coordinates can be optimized [20]. This method usually provides the fastest way of finding the lowest energy structure and this is the only scheme that supports cell optimization in CASTEP. The main advantage of the BFGS minimizer is the ability to perform cell optimization, including optimization at fixed external stress. Elastic constants are evaluated by calculating the stress tensor for a number of distorted structures. Internal coordinates are optimized in each run while keeping the lattice parameters fixed. The accuracy of the elastic constants depends to a great extent on the accuracy of the SCF setting and the level of convergence of geometry optimizations for each distorted structure. These parameters such as the energy cut off, maximum displacement, SCF convergence criteria and k-point set recommended by CASTEP were adopted in calculation, which have balanced the efficiency and precision.

3. Structures formation energies and elastic constants of uranium metal

In order to verify the relevance of the scheme employed in present study, the properties of α-U in ground-state, i.e. one or zero atmospheric pressure and 0 K, were first calculated. The calculated results were then compared with the experimental observations as well as with other theoretical prediction. The α-U structure is fco and there are two atoms in the primitive cell. In Cartesian coordinates, the primitive lattice vectors are given by ($a/2$, $b/2$, 0), ($a/2$, $-b/2$, 0), and (0, 0, c), where a, b, and c are the lattice constants of the conventional unit cell. The two atoms locate at (0, 0, 0) and (0, y, 0.5), where y is the fractional coordinate of the two atoms [3]. The lattice constants experimentally measured at 42 K are 2.836, 5.866, 4.935 Å, and the fraction coordinate y is 0.102 [21]. In present study, these parameter are calculated to be 2.811, 5.913, 4.894 Å and 0.098, matching well with the experimental observations. Söderlind and Boettger et al. have ever calculated the structural parameters of α-U by using the full potential version of the linear muffin-tin orbital (FP-LMTO) method [3,4]. Table 1 shows the comparison of the ground-state properties of α-U calculated by first principles calculations and the corresponding values obtained in experiments [3–5,22–25]. The agreement between experiment and the calculated results is considerably impressive. In addition to the structural parameters of α-U, the elastic constants were also calculated in present study and the calculated results are listed in Table 2. Generally speaking, the elastic constants calculated in present study are more reasonable than those obtained by Söderlind and Randolph et al. [4,13], suggesting that the scheme employed in present study is relevant to investigate the structures and elastic constants of uranium metal. The structural and elastic properties of high temperature phase γ-U, i.e. bcc-U, and hypothetic fcc-U, hcp-U and body-centered tetragonal, i.e. bct-U were also investigated in present study. The bct-U is of particular interest because it has been predicted that this phase might be observed at high pressure [22–25]. Table 3 shows the calculated lattice constants and formation energies of these structures. The formation energy of bcc-U, for example, is computed by $\Delta E_{\mathrm{bcc}}^{\mathrm{for}} = E_{\mathrm{bcc}} - E_{\alpha\text{-U}}$, where E_{bcc} and $E_{\alpha\text{-U}}$ are respectively the total energies of bcc-U and α-U that acquired by first principles calculations in present study. Clearly, the formation energies of these structures are all positive, indicating that they are all less stable than α-U in the ground state. The formation energy of fcc-U is 0.385 eV/atom, the largest one among these structures, showing that the fcc-U is the most unstable among them. The second large one, 0.369 eV/atom, is the formation energy of the ideal hcp-U (i.e. whose $c/a = 1.633$). However, for the full optimized hcp-U, whose $c/a = 1.85$, the formation energy decreases considerably from 0.369 down to 0.233 eV/atom. From Table 3, it could be deduced that the order of stability of these structures in the ground state is, from most stable to most unstable, α, bct, hcp, bcc, ideal hcp and fcc. This conclusion is also supported by other works [3,4,22]. For instance, Boettger et al. found that bcc-U is more stable than fcc-U in ground state.

It is known that the β-U is tetragonal and there are 30 atoms per unit cell. According the geometrical environment, such as the bond length, the 30 atoms can be classified into five types. However, the exact arrangement of these atoms has been a controversial question for long time [6–9,28–35]. At the early stage of 1980s, the controversy resolved itself as to which of the three possible space group is correct: no. 102 ($P\bar{4}n2$), 118 ($P4_2nm$) or 136 ($P4_2/mnm$) (see Table 4). The space group no. 118 has not been seriously considered and the reason for this omission has never been explained. The space group no. 102 was originally favored by Tucker [6,7], but later dropped in favor of the group no. 136 by Tucker and Senio [9,28]. By analogy with the σ-phase, the space group no. 102 was first preferred by Dickins et al. [29], but the space group no. 136 was later preferred by them [30]. Conversely, the analogy with the σ-phase was initially used to favor for β-U [31]. Donohue has ever reviewed the three possible structures and yet obtained no result pointed to one of them being correct [32–34]. Based on the profile refinements of neutron diffract data, Lawson and Olsen argued in 1988 that the symmetry of β-U should be the space group 136 [35]. Since then, to our knowledge, there is no new work has been done for the structure of β-U. In present study, we intend to clarify the precise structure of β-U by using first principles calculations. Accordingly, the structural and elastic properties of all the three possible models were investigated thoroughly.

The three possible structures of β-U were first optimized by using CASTEP and the optimized structural parameters are presented in Table 5. The corresponding parameters obtained from the refinement of experimental data are also listed in this table. One can see that the ab initio calculated structural parameters match considerably well with the experimental observations. Especially, the calculated fractional coordinates are all very close to the data obtained by Lawson. Besides, all the parameters of the three structures are consistent with each other. In particular, due to the restriction of symmetry, some parameters such as x_{II} and y_{III}, for example, are required to have special values in space group no. 136. One notes that such parameters optimized in space groups no. 102 and 118 are also very close to each other and they are all equal to the corresponding special values in the space group no. 136. This observation leads to the supposition of Donohue that the space group of β-U should be the centrosymmetric $P4_2/mnm$, i.e. the space group no.136. In addition, it can be found that the structural parameters of space groups no.136 and 118 acquired by ab initio calculated are totally identical. In fact, from the formulae given in Table 4, one can immediately deduce that the three structures defined by space groups no. 136, 118 and 102 are totally same when the following relations hold: $x_{\mathrm{II}}^{102} = x_{\mathrm{II}}^{118} = x_{\mathrm{II}}^{136}$, $z_{\mathrm{II}}^{102} = 0$, $x_{\mathrm{IIIa}}^{102} = x_{\mathrm{III}}^{118} = x_{\mathrm{III}}^{136} = y_{\mathrm{III}}^{118}$, $z_{\mathrm{IIIa}}^{102} = z_{\mathrm{III}}^{118} = z_{\mathrm{III}}^{136}$, $x_{\mathrm{IIIb}}^{102} = 1 - x_{\mathrm{IIIa}}^{102}$, $z_{\mathrm{IIIb}}^{102} = 1 - z_{\mathrm{IIIa}}^{102}$, $x_{\mathrm{IV}}^{102} = x_{\mathrm{IV}}^{118} = x_{\mathrm{IV}}^{136}$, $y_{\mathrm{IV}}^{102} = y_{\mathrm{IV}}^{118} = y_{\mathrm{IV}}^{136}$, $z_{\mathrm{IV}}^{102} = z_{\mathrm{IV}}^{118} = 0$, $x_{\mathrm{V}}^{102} = x_{\mathrm{V}}^{118} = x_{\mathrm{V}}^{136}$, $y_{\mathrm{V}}^{102} = y_{\mathrm{V}}^{118} = y_{\mathrm{V}}^{136}$, $z_{\mathrm{V}}^{102} = z_{\mathrm{V}}^{118} = 0$. Table 5 shows that these relations indeed hold for the structures defined by space groups no. 136 and 118, though they vary a little for space group no. 102. Accordingly, one can consider that the correct description for the structure of β-U could be space groups no. 136 or 118. However, since the symmetry of space group no. 136 is higher than that of no. 118, e.g. it is needed 7 and 10 parameters for space groups no.136 and 118, respectively, to define the structure of β-U, the space group no.136 is the best choice for the β-U [32,35].

Table 1
Comparison of ground-state properties for α-U ab initio calculated and experimental observations. Lattice constants, *a*, *b*, and *c*, and atomic volumes, V_0, are in units of Å. The internal coordination, *y* is dimensionless.

	Ab initio calculated							Experimental	
a	2.811	2.850–2.880	2.845	2.829	2.797–2.800	2.860	2.809	2.857	2.836
b	5.913	5.850–5.950	5.818	5.770	5.867–5.896	5.770	5.447	5.857	5.866
c	4.894	4.850–4.890	4.996	4.950	4.893	5.010	4.996	4.972	4.935
y	0.098	0.093–0.095	0.103	0.100	0.097–0.098	0.104		0.100	0.102
V_0	20.34	18.95–20.51	20.67	20.20	20.07–20.19	20.72	19.03	20.80	20.52
References	Present work	[3]	[4]	[5]	[13]	[23]	[25]	[1]	[25]

Table 2
Comparison of the ab initio calculated and experimental elastic constants, C_{ij} (Mbar), bulk modular, B_0 (Mbar) of α-U.

	Ab initio calculated			Experimental	
C_{11}	2.55	2.20	2.16–2.27	1.99	1.50
C_{22}	2.01	3.20	3.31–3.36	2.09	2.09
C_{33}	3.45	1.50	1.49–1.53	2.88	2.87
C_{44}	1.27	0.93	1.17–1.29	1.40	1.41
C_{55}	1.15	1.20	0.95–0.99	0.90	0.89
C_{66}	0.88	0.50	0.60	0.84	0.85
C_{12}	0.53	0.05	0.29–0.30	0.40	0.28
C_{13}	0.45	1.10	1.41–1.47	0.24	0.35
C_{23}	1.36	1.33	1.47–1.49	1.10	1.12
B_0	1.32	2.20	2.16–2.27		
References	Present work	[4]	[13]	[26] [a]	[27] [b]

[a] Measured at 73 K.
[b] Measured at 43 K.

Therefore, one can conclude that the symmetry of β-U should belong to space group no. 136.

Once determining the precise structure of β-U, the formation energy, elastic constants and bulk modulus can be calculated by using CASTEP. The formation energy of β-U is calculated to be 0.082 eV/atom, much smaller than that of other metastable structures (see Table 3). It suggests that, in the ground state, β-U is relatively more stable than bcc-U, fcc-U, hcp-U and bct-U. The calculated elastic constants and bulk modular are shown in Table 6. For completeness, the corresponding properties of three possible

Table 3
Ab initio calculated lattice constants, *a* and *c* (Å), and formation energies, ΔE^{for} (eV/atom) of bcc-U, fcc-U, hcp-U and bct-U.

	bcc	fcc	Ideal hcp	hcp	bct	Reference
a	3.455	4.443	3.10	2.99	3.72	Present work
c			5.06	5.52	4.61	
	3.36–3.45	4.25–4.44				[3]
	3.460					[4]
	3.430	4.43–4.48				[13]
	3.37–3.46	4.30				[25]
ΔE^{for}	0.278	0.385	0.369	0.233	0.158	present work
	0.250–0.283	0.367–0.488				[3]
	0.156–0.235	0.216–0.336	0.241–0.281		0.09–0.11	[4]
	0.240–0.270	0.350–0.390				[13]
	0.160	0.260				[25]

Table 4
Three possible descriptions of the unit cell of β-U [2,32].

		atom type
Space group $P4_2/mnm$ *(no. 136)*		
2 atoms in 2*b*:	(0,0,0.5); (0.5,0.5,0)	I
4 atoms in 4*f*:	$(x, x, 0)$; $(\bar{x}, \bar{x}, 0)$; $(0.5+x, 0.5-x, 0.5)$; $(0.5-x, 0.5+x, 0)$	II
8 atoms in 8*j*:	(x, x, z); $(\bar{x}, \bar{x}, \bar{z})$; $(0.5+x, 0.5-x, 0.5+z)$; $(0.5-x, 0.5+x, 0.5-z)$ $(\bar{x}, \bar{x}, z)$; $(x, x, \bar{z})$; $(0.5-x, 0.5+x, 0.5+z)$; $(0.5+x, 0.5-x, 0.5-z)$	III
16 atoms in 2 sets of 8*i*:	$(x, y, 0)$; $(y, x, 0)$; $(0.5+x, 0.5-y, 0.5)$; $(0.5-y, 0.5+x, 0.5)$ $(\bar{x}, \bar{y}, 0)$; $(\bar{y}, \bar{x}, 0)$; $(0.5-x, 0.5+y, 0.5)$; $(0.5+y, 0.5-x, 0.5)$	IV, V
Space group $P\bar{4}n2$ *(no. 118)*		
2 atoms in 2*d*:	(0,0,0.5); (0.5,0.5,0)	I
4 atoms in 4*g*:	$(x, x, 0)$; $(\bar{x}, \bar{x}, 0)$; $(0.5+x, 0.5-x, 0.5)$; $(0.5-x, 0.5+x, 0)$	II
24 atoms in 3 sets of 8*i*:	(x, y, z); $(y, x, \bar{z})$; $(0.5+x, 0.5-y, 0.5+z)$; $(0.5-y, 0.5+x, 0.5-z)$ $(\bar{x}, \bar{y}, z)$; $(\bar{y}, \bar{x}, \bar{z})$; $(0.5-x, 0.5+y, 0.5+z)$; $(0.5+y, 0.5-x, 0.5-z)$	III, IV, V
Space group P4nm (no. 102)		
2 atoms in 2*a*:	(0,0,0.5); (0.5,0.5,0)	I
12 atoms in 3 sets of 4*c*:	(x, x, z); $(\bar{x}, \bar{x}, z)$; $(0.5+x, 0.5-x, 0.5+z)$; $(0.5-x, 0.5+x, 0+z)$	II, IIIa, III_b
16 atoms in 2 sets of 8*d*:	(x, y, z); $(y, x, \bar{z})$; $(0.5+x, 0.5-y, 0.5+z)$; $(0.5+y, 0.5-x, 0.5+z)$ $(\bar{x}, \bar{y}, z)$; $(\bar{y}, \bar{x}, \bar{z})$; $(0.5-x, 0.5+y, 0.5+z)$; $(0.5-y, 0.5+x, 0.5+z)$	IV, V

Table 5
Ab initio calculated in present study and experimental [32,35] structural properties of β-U. The origins are moved to place U1 atoms at $x = y = 0$ and $z = 0.5$. Values in brackets, i.e. |0|, are fixed by symmetry. The units of lattice constants, a and c are Å, bulk modulus, B_0, is Mbar. and the others are dimensionless.

	Present work			Experimental [35]			Experimental [32]		
	136	118	102	136	118	102	136	118	102
a	10.520	10.520	10.517	10.759		10.52			
c	5.707	5.707	5.723	5.653		5.57			
x_{II}	0.111	0.111	0.111	0.103	0.103	0.103	0.098–0.103	0.100	0.107–0.110
z_{II}	|0|	|0|	0.027	|0|	|0|	−0.007	|0|	|0|	−0.014–0.070
x_{IIIa}	0.320	0.320	0.321	0.319	0.321	0.319	0.316–0.321	0.313	0.290–0.320
y_{IIIa}		0.320			0.316			0.323	
z_{IIIa}	0.723	0.723	0.721	0.744	0.744	0.746	0.720–0.730	0.725	0.769–0.840
x_{IIIb}			0.680			0.683			0.671–0.690
z_{IIIb}			0.278			0.254			0.294–0.340
x_{IV}	0.556	0.556	0.555	0.562	0.562	0.562	0.556–0.561	0.557	0.547–0.563
y_{IV}	0.236	0.236	0.229	0.234	0.234	0.236	0.214–0.235	0.228	0.220–0.240
z_{IV}	|0|	0.000	0.024	|0|	−0.004	−0.014	|0|	0.043	0.052–0.090
x_{V}	0.364	0.364	0.361	0.366	0.365	0.365	0.367–0.370	0.368	0.367–0.380
y_{V}	0.044	0.044	0.054	0.039	0.040	0.040	0.038–0.046	0.041	0.040–0.045
z_{V}	|0|	0.000	−0.028	|0|	0.007	−0.003	|0|	−0.017	−0.026–0.040

Table 6
Elastic constants, C_{ij} (Mbar), and bulk moduli, B_0 (Mbar), of β-U, γ-U, fcc-U, hcp-U and bct-U ab initio calculated in present study.

	$P4_2/mnm$	$P\bar{4}n2$	$P4_2nm$	bct	hcp	bcc		fcc	
C_{11}	2.18	2.14	2.04	2.30	2.16	1.03	1.61[a]	0.71	1.84[a]
C_{33}	2.14	2.15	2.16	2.04	2.02				
C_{44}	0.60	0.59	0.52	0.79	0.35	0.46	0.56[a]	0.26	0.28[a]
C_{66}	0.61	0.61	0.57	0.39					
C_{12}	0.99	0.99	0.91	0.61	0.80	1.42	1.84[a]	1.44	2.67[a]
C_{13}	0.80	0.79	0.77	0.61	0.58				
B_0	1.30	1.28	1.24	1.14	1.15	1.29		1.11	

[a] Reference [13].

structures of β-U, and γ-U, fcc-U, hcp-U and bct-U were all calculated. It can be found that the calculated elastic constants of β-U described by space group no. 136 are almost the same as that of no. 118. In fact, because the structure of β-U defined by space groups no. 136 and 118 are totally identical, it is naturedly that their elastic constants should be equal to each other.

A crystal may have several elastic constants and those elastic constants may vary significantly from other to another. However, the crystal may still yield an isotropic behavior accidentally. According to Grimvall [36], for example, a crystal with tetragonal symmetry is elastically isotropic if the follow relations hold: $C_{11} = C_{33}$, $C_{12} = C_{13}$ and $C_{44} = C_{66} = (C_{11} - C_{12})/2$. Interestingly, one may found from Table 6 that these relations hold perfectly for β-U. Take the β-U described by space group no. 136 as an example, $(C_{11} + C_{33})/2 - (C_{12} + C_{13})/2 = 1.27$ Mbar, almost equaling to the value of $(C_{44} + C_{66}) = 1.21$ Mbar. Lawson has ever computed the anisotropy of thermal parameters of β-U defined by space group no. 136 and indeed found that the anisotropy was very small [35]. This observation indicates that β-U may exhibit some isotropic behavior. Besides, it can be found that the Zener's shear constants, i.e. $C' = C_{11} - C_{12}$, of bcc-U and fcc-U are negative [36], indicating that these structures can neither stable nor metastable exist mechanically in the ground state, which satisfyingly accounts for the formation energies of bcc-U and fcc U are much larger than those of other structures. These conclusions were also supported by the work of Taylor (see Table 3) [12,13,24,25,34,35].

In the discussion above, one notes that the values of the same structural parameter or physical property obtained by different researcher might vary in a narrow range. Those variations do not only result from the statistic error or experimental fluctuation, but also result from the different experimental conditions, different approximations and algorithms adopted in calculations. Concerning this issue, Boettger, Christopher have investigated these effect of different schemes employed in first principles calculations and found that the structural parameters, formation energies obtained by them did not significantly differ from each other [4,13].

4. Conclusion

The structures and elastic constants of uranium metal, including the α-U, β-U, γ-U, fcc-U, hcp-U and bct-U, were investigated by first principles calculations. The main attention was specially paid to the three possible structures of β-U that described by space groups no. 136, 118 and 102. It turns out that the structures described by the No. 118 and No. 136 can be identical for the β-U and that the correct symmetry of β-U should belong to space group no. 136. Interestingly, the calculated elastic constants show that β-U might exhibit some isotropic behaviors. Besides, both γ-U and fcc-U are unstable in the ground state because their Zener's shear constants are negative. The obtained structure parameters, elastic constants and the formation energies of uranium metal can be used to develop and verify an atomistic potential, providing a basis for future investigating the structural and transformational behaviors of metallic uranium upon dissolving other metal atoms.

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