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Electronic structures and physical properties of pure Cr, Mo and W①

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Abstract: Using the one atom theory, the electronic structures of pure Cr, Mo and W with bcc structure were determined respectively as: $[Ar](3d_c)^{3.32}(3d_n)^{2.26}(4s_c)^{0.25}(4s_f)^{0.17}$, $[Kr](4d_c)^{4.23}(4d_n)^{1.48}(5s_c)^{0.02}(5s_f)^{0.27}$ and $[Xe](5d_c)^{5.16}(6s_c)^{0.25}(6s_f)^{0.59}$. The electronic structures of these metals with hcp and fcc structures and liquid state were also studied. According to their electronic structures, the relationship between the electronic structure and crystalline structure was explained qualitatively and the relationship between the difference of mechanical properties and transport properties of pure Cr, Mo and W with bcc structure and their electronic structures was also explained qualitatively; the lattice constants, binding energy, potential curves, elasticities and the temperature dependence of the linear thermal expansion coefficient of bcc-Cr, bcc-Mo and bcc-W were calculated quantitatively.

Key words: Cr; Mo; W; electronic structure; crystalline structure; lattice constant; binding energy; mechanical property; transport property

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1 INTRODUCTION

In the framework of the metallic materials systematic science[1], there are three scientific theory systems: pure metal systematic science, alloys physics and chemistry, and alloys statistical thermodynamics. The core of the pure metal systemar tic science is the one atom theory (OA)[2-5], and that of the alloys physics and chemistry and alloys statistical thermodynamics is the characteristic crystal theory (CC). In order to make the materials design step from empirical to scientific under the guidance of the metallic materials systematic science, the first step is to establish a pure metal data base according to OA theory. Using the auto-search-solution OA theory program developed by the authors, the calculation for electronic structures and physical properties of pure metal Cr, Mo, W, Pt, Ru, etc have been completed, and that of Cr, Mo, W are introduced in this paper.

2 BASIC ATOM STATES OF Cr, Mo AND W

In the OA theory, the electronic structures of pure metals are described by the quasi-electron-occupation(QEO) number of the one-atom state Ψ_a which is made up of some basic atom states φ_k:

$$\psi_a = \sum_k c_k \phi_k \quad (1)$$

At the outer shell of Cr, Mo, W atom, there are covalent electrons n_c, near-free electrons n_f and no-bond electrons n_n. In each basic atom state, the distribution of electrons follows the Pauli exclusion principle.

The characteristic properties(lattice constant a and binding energy E_c) of the pseudo-crystals formed by atoms in each kind of basic atom state of Cr, Mo, W metal can be obtained using a series of established expressions[3]. The results of Cr metal are listed in Table 1.

3 ELECTRONIC STRUCTURES OF Cr, Mo, W

3.1 Electronic structures of bcc-Cr, bcc-Mo and bcc-W

In our research, firstly we take the two characteristic properties(a and E_c) as the criterion and perform the three-state hybridization to all the 17 basic atom states with the step length of 0.01. Secondly, after a systematic analysis mainly taking the lattice constants and binding energies into consideration, the three-state combination of bcc-Cr, bcc-Mo and bcc-W are determined as follows:

$c_2 = 0.04$, $c_{12} = 0.79$, $c_{14} = 0.17$;

$c_4 = 0.27$, $c_{12} = 0.72$, $c_{13} = 0.01$;

$c_1 = 0.17$, $c_3 = 0.25$, $c_6 = 0.58$.

Then the electronic structures of bcc-Cr, bcc-Mo and bcc-W are determined as

$$\Psi_a(\text{bcc-Cr}) = [Ar](3d_c)^{3.32}(3d_n)^{2.26}(4s_c)^{0.25} \cdot (4s_f)^{0.17};$$

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Ψ_a (bcc-Mo) = [Kr] $(4d_c)^{4.23}$ $(4d_n)^{1.48}$ · $(5s_c)^{0.02}(5s_f)^{0.27}$;

Ψ_a(bcc-W) = [Xe] $(5d_c)^{5.16}(6s_c)^{0.25}(6s_f)^{0.59}$.

This process of determining electronic structure is multiple-properties-determining-state method in OA theory[6]. The atom state parameters, bond parameters and characteristic properties of bcc-Cr, bcc-Mo and bcc-W crystal are listed in Table 2, where r_1, r_2, r_3 and n_1, n_2, n_3 denote covalent bond length and covalent electron pair number, respectively.

3.2 Electronic structures of hcp-Cr, fcc-Cr, hcp-Mo, fcc-Mo, hcp-W and fcc-W

3.2.1 Binding energies of hcp-Cr, fcc-Cr, hcp-Mo, fcc-Mo, hcp-W and fcc-W

Under the isopiestic condition, the Gibbs energy of pure metal is a function of specific heat capacity $C_p(T)$ and volume $V(T)$:

$$G(T) = E_c + \int_0^T C_p(T)\,dT + p\int_0^T V(T)\,dT - T\int_0^T C_p(T)/T\,dT \quad (2)$$

where p is pressure and T is temperature.

The relative Gibbs energy is presented by a polynomial of T in SGTE(Scientific Group Thermodata, Europe) database[7]:

$$G'(T) = a + bT + cT\ln T + \sum k_n T^n \quad (3)$$

where $G'(T)$ is the relative Gibbs energy, and it is not equal to $G(T)$. At 0 K, there exists

$$G(T) - G'(T) = E_c - a \quad (4)$$

Table 1 Basic atom states and corresponding pseudo-crystal characteristic properties of Cr

k	Electronic structure in outer shell	a/nm			E_c/(kJ·mol^{-1})		
		bcc	hcp	fcc	bcc	hcp	fcc
1	$(3d_c)^4(3d_n)^0(4s_c)^0(4s_f)^2$	0.310 08	0.275 53	0.389 68	371.75	367.31	362.04
2	$(3d_c)^4(3d_n)^0(4s_c)^2(4s_f)^0$	0.298 15	0.265 00	0.374 79	650.78	645.17	644.96
3	$(3d_c)^4(3d_n)^0(4s_c)^1(4s_f)^1$	0.303 51	0.269 74	0.381 49	515.18	510.53	508.23
4	$(3d_c)^5(3d_n)^0(4s_c)^0(4s_f)^1$	0.284 71	0.253 13	0.358 01	502.66	498.52	496.01
5	$(3d_c)^5(3d_n)^0(4s_c)^1(4s_f)^0$	0.279 36	0.248 40	0.351 33	706.47	701.07	700.69
6	$(3d_c)^6(3d_n)^0(4s_c)^0(4s_f)^0$	0.260 62	0.231 82	0.327 90	689.69	685.05	684.46
7	$(3d_c)^2(3d_n)^2(4s_c)^0(4s_f)^2$	0.358 80	0.318 88	0.450 98	176.27	174.39	168.03
8	$(3d_c)^2(3d_n)^2(4s_c)^2(4s_f)^0$	0.328 94	0.292 16	0.413 19	375.51	371.83	371.75
9	$(3d_c)^2(3d_n)^2(4s_c)^1(4s_f)^1$	0.337 43	0.306 42	0.433 37	271.54	262.46	260.04
10	$(3d_c)^3(3d_n)^2(4s_c)^0(4s_f)^1$	0.309 14	0.281 53	0.398 20	276.81	267.11	264.39
11	$(3d_c)^3(3d_n)^2(4s_c)^1(4s_f)^0$	0.300 67	0.267 23	0.377 94	436.31	432.50	432.37
12	$(3d_c)^4(3d_n)^2(4s_c)^0(4s_f)^0$	0.272 49	0.242 33	0.342 75	440.41	437.19	436.94
13	$(3d_c)^0(3d_n)^4(4s_c)^2(4s_f)^0$	0.415 41	0.368 76	0.521 52	65.10	64.39	64.39
14	$(3d_c)^0(3d_n)^4(4s_c)^1(4s_f)^1$	0.439 69	0.390 11	0.551 70	45.27	44.73	42.13
15	$(3d_c)^1(3d_n)^4(4s_c)^0(4s_f)^1$	0.382 97	0.340 19	0.481 12	82.68	81.76	78.78
16	$(3d_c)^1(3d_n)^4(4s_c)^1(4s_f)^0$	0.358 80	0.318 88	0.450 98	171.71	170.20	170.16
17	$(3d_c)^2(3d_n)^4(4s_c)^0(4s_f)^0$	0.302 51	0.269 11	0.380 65	197.90	196.65	196.44

Table 2 Atom state parameters, bond parameters and characteristic properties of bcc-Cr, bcc-Mo, bcc-W crystal

	Atom state parameter				Bond parameter							Theor.		Exptl.	
	d_c	d_n	s_c	s_f	R/nm	r_1/nm	r_2/nm	r_3/nm	n_1	n_2	n_3	a/nm	E_c/(kJ·mol^{-1})	a/nm[8]	E_c/(kJ·mol^{-1})[9]
bcc-Cr	3.32	2.26	0.25	0.17	0.11231	0.249 83	0.288 48	0.407 97	0.380 2	0.091 5	0.000 9	0.288 48	395.35	0.288 46	395
bcc-Mo	4.23	1.48	0.02	0.27	0.126 20	0.272 54	0.314 70	0.445 05	0.461 7	0.091 5	0.000 6	0.314 70	658.26	0.314 66	658
bcc-W	5.16	0	0.25	0.59	0.130 19	0.274 20	0.316 62	0.447 77	0.588 5	0.115 5	0.000 8	0.316 62	858.33	0.316 52	859

According to the binding energies of bcc-Cr, bcc-Mo, bcc-W and the $G'(T)$ data of bcc-Cr, hcp-Cr, fcc-Cr, bcc-Mo, hcp-Mo, fcc-Mo, bcc-W, hcp-W, fcc-W supplied in SGTE database, the binding energies of hcp-Cr, fcc-Cr, hcp-Mo, fcc-Mo, hcp-W and fcc-W are obtained approximately as follows:

E_c(hcp-Cr) = 390.56 kJ/mol, E_c(fcc-Cr) = 387.71 kJ/mol; E_c(hcp-Mo) = 646.45 kJ/mol, E_c(fcc-Mo) = 642.80 kJ/mol, E_c(hcp-W) = 844.25 kJ/mol, E_c(fcc-W) = 839.70 kJ/mol.

3.2.2 Lattice constants of hcp-Cr, fcc-Cr, hcp-Mo, fcc-Mo, hcp-W and fcc-W

As the experimental lattice constants of hcp-Cr, fcc-Cr, hcp-Mo, fcc-Mo, hcp-W and fcc-W can not be obtained, we use the method similar to Ref. [10], that is, supposing Cr, Mo, W metals with hcp and fcc structures have the same atom volume as those with bcc structure. Therefore, the lattice constants of hcp-Cr, fcc-Cr, hcp-Mo, fcc-Mo, hcp-W and fcc-W are obtained approximately as follows:

a(hcp-Cr) = 0.256 99 nm, a(fcc-Cr) = 0.363 44 nm; a(hcp-Mo) = 0.280 35 nm, a(fcc-Mo) = 0.396 45 nm; a(hcp-W) = 0.281 99 nm, a(fcc-W) = 0.398 79 nm.

3.2.3 Electronic structures of hcp-Cr, fcc-Cr, hcp-Mo, fcc-Mo, hcp-W and fcc-W

Similar to determining the electronic structures of bcc-Cr, bcc-Mo and bcc-W, electronic structures of hcp-Cr, fcc-Cr, hcp-Mo, fcc-Mo, hcp-W and fcc-W can be determined by the multiple-properties-determining-state method as

$$\Psi_a(\text{hcp-Cr}) = [\text{Ar}](3d_c)^{3.24}(3d_n)^{2.40}(4s_c)^{0.28}\cdot(4s_f)^{0.08},$$

$$\Psi_a(\text{fcc-Cr}) = [\text{Ar}](3d_c)^{3.14}(3d_n)^{2.54}(4s_c)^{0.32};$$

$$\Psi_a(\text{hcp-Mo}) = [\text{Kr}](4d_c)^{4.00}(4d_n)^{1.74}\cdot(5s_c)^{0.09}(5s_f)^{0.17},$$

$$\Psi_a(\text{fcc-Mo}) = [\text{Kr}](4d_c)^{3.79}(4d_n)^{2.00}\cdot(5s_c)^{0.17}(5s_f)^{0.04};$$

$$\Psi_a(\text{hcp-W}) = [\text{Xe}](5d_c)^{4.88}(5d_n)^{0.32}(6s_c)^{0.40}\cdot(6s_f)^{0.40},$$

$$\Psi_a(\text{fcc-W}) = [\text{Xe}](5d_c)^{4.50}(5d_n)^{0.82}(6s_c)^{0.61}\cdot(6s_f)^{0.07}.$$

3.2.4 Electronic structures of liquid metals L-Cr, L-Mo and L-W

Similar to the case of hcp-Cr, fcc-Cr, hcp-Mo, fcc-Mo, hcp-W and fcc-W, the binding energies of L-Cr, L-Mo and L-W are determined through SGTE database as follows:

E_c(L-Cr) = 370.66 kJ/mol; E_c(L-Mo) = 616.17 kJ/mol; E_c(L-W) = 806.84 kJ/mol.

Supposing Cr, Mo, W still have bcc structure after being melted, according to their densities[11] before and after being melted and the lattice constants of solid bcc-Cr, bcc-Mo, bcc-W, the lattice constants of L-Cr, L-Mo and L-W are obtained as follows:

a(L-Cr) = 0.301 45 nm, a(L-Mo) = 0.324 36 nm, a(L-W) = 0.325 53 nm. By the way, it has been confirmed by modern X-ray experiments that liquid metals really have the short distance ordering similar to crystals.

Similar to the case above, the electronic structures of L-Cr, L-Mo and L-W are obtained as:

$$\Psi_a(\text{L-Cr}) = [\text{Ar}](3d_c)^{3.44}(3d_n)^{1.52}(4s_c)^{0.20}(4s_f)^{0.84};$$

$$\Psi_a(\text{L-Mo}) = [\text{Kr}](4d_c)^{4.00}(4d_n)^{1.36}(5s_c)^{0.08}(5s_f)^{0.56};$$

$$\Psi_a(\text{L-W}) = [\text{Xe}](5d_c)^{4.69}(6s_c)^{0.50}(6s_f)^{0.81}.$$

4 QUALITATIVE EXPLANATION OF RELATIONSHIP BETWEEN CRYSTALLINE STRUCTURES AND ELECTRONIC STRUCTURES OF Cr, Mo AND W

Compared with various kinds of first-principle methods, an important feature of the description of the electronic structure in OA theory is the function division of electrons in outer shells. On the basis of this, a qualitative explanation about why the crystalline structures of metals exist can be presented.

In the full p^6 shells of Cr, Mo and W metals, electron cloud of p orbits extends along x, y and z axes. Along these directions, the shield effect of electrons to nuclear charges is the strongest, while between the axes the effect is weaker. So, there are two direction systems with weak shield effect outside p^6 shell[5]. The first direction system is ⟨111⟩ directions along 4 body diagonal lines, and the angle between them and p_x, p_y and p_z is the biggest (54.75°). The second is ⟨110⟩ directions along 3 pairs of diagonal lines on xy, yz and xz planes, and the corresponding angle is 45°.

The d electrons out of p^6 shell are divided into e_g and t_{2g}, and they have different energy and symmetry: d electrons with e_g state extend along ⟨111⟩ directions (that is, the first direction system mentioned above), and those with t_{2g} extend along the ⟨110⟩ directions (that is, the second direction system mentioned above). d electrons first fill e_g orbits with low energy, and bonds along ⟨111⟩ directions are formed. Atoms with this state are inclined to form bcc structure crystal with low symmetry. With the increase of d_c electrons with e_g state, the bcc structure becomes more stable. s electrons are sphere symmetrical, their existence is favorable to forming crystalline structures with high symmetry. The coordination number of bcc structure is 8, and that of hcp and fcc structure are 6+6 (the nearest number+the next nearest number), 12 respectively. That is, from bcc to hcp to fcc, the bond directivity becomes weaker and the symmetry becomes stronger. The calculation results of electronic structures in our study can give a satisfactory explanation about why the crystalline structures of Cr, Mo, W metals exist. In the course

of bcc → hcp → fcc, d_c electrons become less gradually (Cr: 3.32 → 3.24 → 3.14; Mo: 4.23 → 4.00 → 3.79; W: 5.16 → 4.88 → 4.50), while s_c electrons become more gradually (Cr: 0.25 → 0.28 → 0.32; Mo: 0.02 → 0.09 → 0.17; W: 0.25 → 0.40 → 0.61). This makes the symmetry of the electron cloud distribution become stronger, so the coordination number becomes larger.

5 QUALITATIVE EXPLANATION OF RELATIONSHIP BETWEEN DIFFERENCE OF PHYSICAL PROPERTIES OF Cr, Mo, W METALS AND THEIR ELECTRONIC STRUCTURES

Based on the function division of outer-shell electrons, not only the relationship between the existence of the crystalline structures of Cr, Mo, W metals and their electronic structures, but also the relationship between the difference of physical properties of Cr, Mo, W metals and their electronic structures can be explained qualitatively. In order to compare with experimental results, only Cr, Mo and W with bcc structure are presented here.

Generally, the following two kinds of properties of metals are always taken into account: one is the mechanical properties (including elasticity, strength, tenacity, hardness and brittleness), the other is transport properties (including electrical conductivity, thermal conductivity). From the viewpoint of condensed physics, mechanical properties are the embodiment of combination properties of metal crystals in essence. In OA theory, outer-shell electrons of metal atoms are divided into 4 kinds: covalent electrons n_c, near-free electrons n_f, no-bond electrons n_n and magnetic electrons n_m. Covalent electrons n_c are responsible for forming the bond network to bind metal atoms. It can be considered that the more the covalent electrons are, the stronger the binding is, and the greater the strength and hardness are. Furthermore, a mechanical property parameter $M = n_c$ can be introduced to describe the binding strength of metal crystals. The M data, tensile strength, Vickers hardness, bulk modulus and melting point of Cr, Mo, W metals are listed in Table 3. It can be seen that their change trends are the same.

It must be pointed out that structure-sensitive properties such as strength and hardness are connected with many factors. The organization and structure of the specimen (monocrystalline, polycrystalline, size of crystal grains), the product form of the specimen (cast product, forging part, rolled product, extruded section and P/M product), heat processing technology (quenching, annealing, annealing temperature, annealing time), the shape and size of the specimen (rod, sheet), test conditions (strain rate, temperature) can all affect experimental results greatly. So the decentralization rate of the experimental data from various sources is great, and their comparability is bad. As a kind of structure-insensitive property, the comparability of bulk modulus data is much better. Furthermore, although melting point is usually not considered as a kind of mechanical property, it can be a very good parameter to describe the binding strength of metal crystals. It can be measured precisely, and the decentralization rate of results is small. So, the melting points are also listed in Table 3.

Table 3 Relationship between difference of mechanical properties and transport properties of Cr, Mo, W metals with bcc structure and their electronic structures

Property	Metal		
	bcc-Cr	bcc-Mo	bcc-W
M	3.57	4.25	5.41
Tensile strength/MPa[8]	282	300	380
Vickers hardness[8]	135	180	190
Bulk modulus/GPa[9]	190.1	272.5	323.2
Melting point/K[8]	2148	2883	3683±20
T'/nm^{-3}	14.16	17.33	37.21
$\sigma_{295\,K}$/10^{-5}($\Omega^{-1}\cdot$cm^{-1})[9]	0.78	1.89	1.89
$K_{300\,K}$/(W·cm^{-1}·K^{-1})[9]	0.94	1.38	1.74

According to the solid electronic theory in condensed physics, the expressions of the electrical conductivity σ and thermal conductivity K are as follows[9]:

$$\sigma = \frac{ne^2\tau}{m} \tag{5}$$

$$K = \frac{\pi^2 n k_B^2 T \tau}{3m} \tag{6}$$

where n is electron concentration, e is electron charge, τ is relaxation time, m is electron mass, k_B is Boltzmann constant, T is Kelvin temperature. As e, m, k_B are all constants, if we assume that the relaxation time τ of Cr, Mo and W are the same, the electrical conductivity σ and thermal conductivity K of Cr, Mo, W will be in direct proportion to the electron concentration n at the same temperature.

In OA theory, near-free electrons in outer shells of metal atoms are responsible for transporting electricity and heat. A parameter of transport property $T' = n_f/V$ can be introduced to describe the transport property of metals, where V is the atom volume. It can be seen that the physical meaning of the transport property parameter is the near-free electrons

concentration. The transport properties parameter T', electrical conductivity γ and thermal conductivity K are also listed in Table 3. It can be seen that their change trends are also the same.

6 QUANTITATIVE CALCULATIONS OF PHYSICAL PROPERTIES OF Cr, Mo AND W WITH BCC STRUCTURE

Seen as a whole, one of the critical parts of OA theory is the determination of electronic structure, the other is the qualitative explanations and quantitative calculations of various physical properties based on the electronic structures obtained above. The object of researching electronic structure is to perform these kinds of explanations and calculations, and to understand the change rules of various physical properties in essence and control them effectively. On the other hand, these kinds of qualitative explanations and calculations can also be used to judge whether the electronic structures are proper or not. The potential curves, elasticity and the changes of linear thermal expansion with temperature of Cr, Mo and W with bcc structure are calculated here. It is necessary to point out that these calculations can also be performed to Cr, Mo and W with hcp and fcc structures and liquid state. Only calculation results of Cr, Mo and W with bcc structure are presented here, because it is convenient to compare them with experimental results.

6.1 Theoretical potential curves

According to many-atom interactions(MAI) potential function, the theoretical potential curves of Cr, Mo and W with bcc structure are shown in Fig. 1.

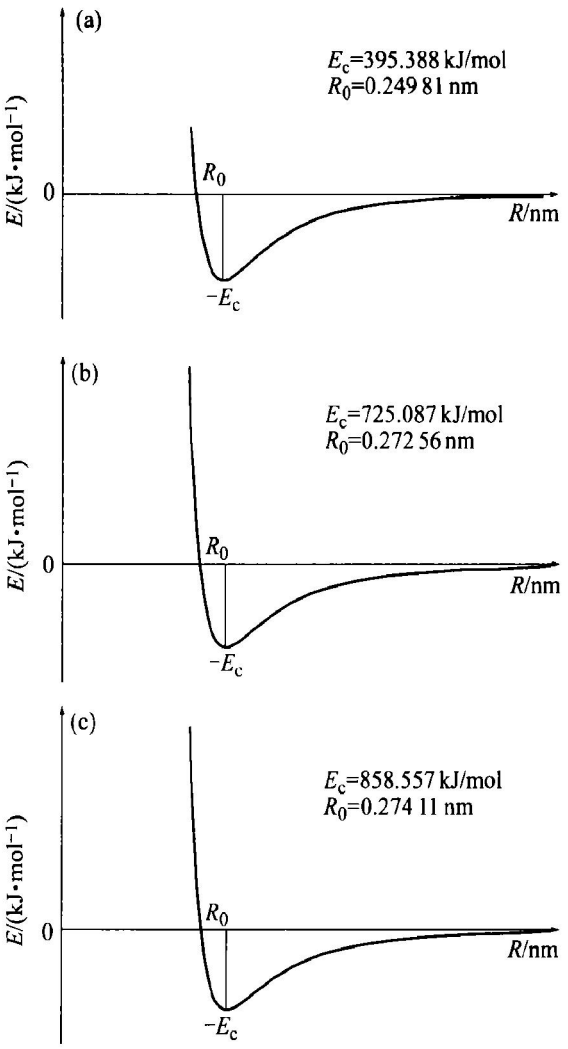

Fig. 1 Theoretical potential curves of bcc-Cr(a), bcc-Mo(b) and bcc-W(c)

6.2 Elasticity

According to the elasticity calculation formula in OA theory, bulk modulus(B), elastic modulus(Y), modulus rigidity(μ) and Poisson's ratio(γ) of bcc-Cr, bcc-Mo and bcc-W are listed in Table 4.

6.3 Linear thermal expansion coefficient as a function of temperature for bcc-Cr, bcc-Mo and bcc-W

According to the expression between linear thermal expansion coefficient and temperature in OA theory, the change curves of linear thermal expansion coefficient as a function of temperature of bcc-Cr, bcc-Mo and bcc-W are shown in Fig. 2.

Table 4 Elasticities of bcc-Cr, bcc-Mo and bcc-W

Elasticity	bcc-Cr		bcc-Mo			
	Theor.	Exptl.	Theor.	Exptl.	Theor.	Exptl.
B/GPa	184	190.1[9]	272	272.5[9]	316	323.2[9]
Y/GPa	187		276		321	
μ/GPa	70		104		121	
γ	0.3308		0.3308		0.3308	

7 CONCLUSIONS

1) When Cr, Mo and W atoms get together, there are 0.58, 0.71 and 0.16 s electrons transforming into d electrons respectively. So, the electronic structures of bcc-Cr, bcc-Mo and bcc-W can be described as follows: $\Psi_a(\text{bcc-Cr}) = [\text{Ar}]\cdot(3d_c)^{3.32}(3d_n)^{2.26}(4s_c)^{0.25}(4s_f)^{0.17}$, $\Psi_a(\text{bcc-Mo}) = [\text{Kr}](4d_c)^{4.23}(4d_n)^{1.48}(5s_c)^{0.02}(5s_f)^{0.27}$, $\Psi_a(\text{bcc-W}) = [\text{Xe}](5d_c)^{5.16}(6s_c)^{0.25}(6s_f)^{0.59}$.

2) Based on the electronic structures of Cr, Mo and W, the relationship between their crystalline structures and electronic structures is explained qualitatively; the relationship between the difference of the physical properties of Cr, Mo and W with bcc structure and their electronic structures is explained qualitatively; the lattice constants, binding energies,

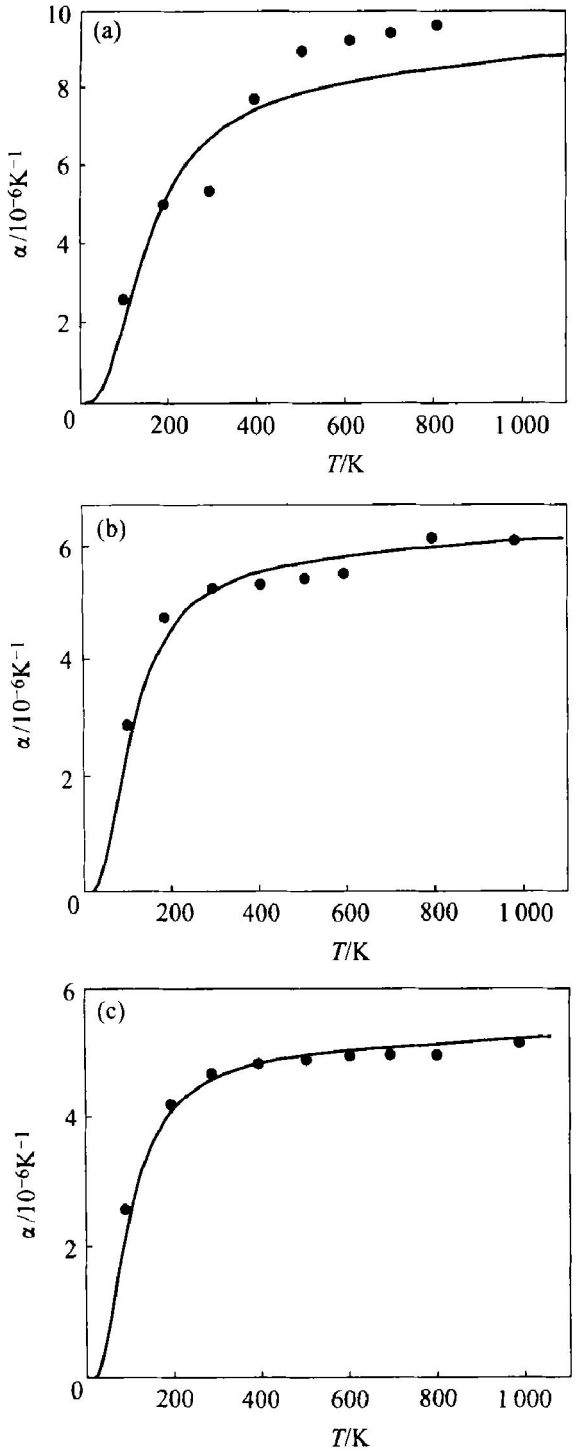

Fig. 2 Linear thermal expansion coefficient as a function of temperature for bcc-Cr(a), bcc-Mo(b), bcc-W(c) (• —Exptl. values[12])

potential curves, elasticity and change curves of linear thermal expansion coefficient as a function of temperature are calculated quantitatively, and the theoretical values and experimental values are in good accordance.

3) Electronic structures of hcp-Cr, fcc-Cr, L-Cr, hcp-Mo, fcc-Mo, L-Mo, hcp-W, fcc-W, L-Cr, L-Mo and L-W are obtained as follows: Ψ_a(hcp-Cr) = [Ar] $(3d_c)^{3.24}(3d_n)^{2.40}(4s_c)^{0.28}\cdot(4s_f)^{0.08}$, Ψ_a(fcc-Cr) = [Ar] $(3d_c)^{3.14}(3d_n)^{2.54}\cdot(4s_c)^{0.32}$, Ψ_a(L-Cr) = [Ar] $(3d_c)^{3.44}(3d_n)^{1.52}\cdot(4s_c)^{0.20}(4s_f)^{0.84}$; Ψ_a(hcp-Mo) = [Kr] $(4d_c)^{4.00}\cdot(4d_n)^{1.74}(5s_c)^{0.09}(5s_f)^{0.17}$, Ψ_a(fcc-Mo) = [Kr] $(4d_c)^{3.79}(4d_n)^{2.00}(5s_c)^{0.17}(5s_f)^{0.04}$, Ψ_a(L-Mo) = [Kr] $(4d_c)^{4.00}(4d_n)^{1.36}(5s_c)^{0.08}(5s_f)^{0.56}$; Ψ_a(hcp-W) = [Xe] $(5d_c)^{4.88}(5d_n)^{0.32}(6s_c)^{0.40}\cdot(6s_f)^{0.40}$, Ψ_a(fcc-W) = [Xe] $(5d_c)^{4.50}(5d_n)^{0.82}\cdot(6s_c)^{0.61}(6s_f)^{0.07}$, Ψ_a(L-W) = [Xe] $(5d_c)^{4.69}\cdot(6s_c)^{0.50}(6s_f)^{0.81}$.

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