First-principles investigations of structural, elastic, thermodynamic and electronic properties of Pt₃Hf compound under pressure

Zongbo Li¹,², Kai Xiong¹,²*, Yingjie Sun¹, Xiuhua Chen¹, Junjie He¹, Shunmeng Zhang¹, Yingjie Fu¹, Yong Mao¹,²*

1 School of Materials Science and Engineering, Yunnan Provincial Engineering Laboratory of Copper-based and Advanced Conductive Materials, Yunnan University, Kunming 650091, China.
2 Materials Genome Institute of Yunnan University, Yunnan University, Kunming 650091, China.
E-mail: xiongkai@ynu.edu.cn, maoyong@ynu.edu.cn

Abstract. The pressure effects on the structure, elasticity, thermodynamics and electronic properties of Pt₃Hf compounds were investigated by first-principles calculations based on density functional theory. The obtained equilibrium lattice parameter is consistent with the experimental and theoretical values. The calculation results show that the elastic constants, bulk modulus, shear modulus, Young modulus, anisotropy factor and Debye temperature, sound velocities increase with the increase of pressure. The B/G ratio and Poisson’s ratio results show an upward trend with increasing pressure, which means that increasing external pressure can enhance the ductility of Pt₃Hf compound. Analyzing the charge density difference and the density of states reveal that charge accumulation gradually increases with the increase of pressure between Pt and Hf atoms.

1. Introduction

Platinum group metal alloys (PGMs) have attract great attentions because of their have high melting point, superior oxidation high specific strength, and corrosion resistance [1], which means that it important in high temperature structural materials applications field. Especially, the high-strength properties of Pt-based intermetallic compounds is far beyond the traditional Ni-based super-alloys [2]. Among Pt-based alloys, Pt₃Hf intermetallic compound has attract physical properties on both on industrial and high-temperature field. Among them, Pt₃Hf compound is an L1₂ structure with good mechanical properties in
high temperature structural materials.

It is well known that pressure plays an important character in the mechanical, elastic, thermodynamic and electronic properties of material performances[3]. Therefore, studying the elastic properties of PtHf intermetallic compounds under extreme high pressures conditions is of great significance for Pt-based alloys. However, there are few reports on the experimental and electronic calculations of the structural properties of PtHf intermetallic compounds at high pressure. Investigations on the structure, elasticity, thermodynamic and electronic properties of PtHf compound under high pressure are valuable and urgently needed for its high-temperature applications. For PtHf, the previous studies mainly investigated the mechanical properties elastic constant elastic modulus at zero GPa. POPOOLA et al. [4] And the investigations of high temperature thermodynamic properties in Pt-HF systems for published paper [5]. Because it is difficult to achieve and control under the experimental conditions under high pressure, but can easily achieved under simulated conditions to provide some guidance for the experiment. However, there are no literature reports on experimental or theoretical studies on the structure, elasticity, thermodynamics and electronic properties of PtHf intermetallic compounds under high pressure.

Thus, it is very urgent and meaningful to investigate the mechanical and thermodynamic properties of PtHf intermetallic compound with pressure. In this paper, we focus on the structure, elastic, electronic and thermodynamic properties of PtHf intermetallic compound under high pressure (from 0–100 GPa).

2. Computational method

The calculations were performed within the frame of density function theory (DFT) by using the Vienna plane wave ab initio simulation package (VASP) [6]. Using the projector augmented wave method, (PAW) [7] exchange-correlation functional was treated by the generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) [8]. The atoms basis PAW was selected on 5d6s for Pt and 5d6s for Hf. The kinetic cut-off energy of 500 eV was shown an excellent convergence of the total energies and structural parameters. The Brillouin zones of the unit cells were represented by the 9×9×9, 15×15×15 Monkhorst-Pack grid meshes. The energy change was converged to lower than 1.0×10^-5 eV, and the maximum force less than 0.01 eV/Å.

3. Results and discussion

3.1 Structural properties

The PtHf intermetallic compound belongs to the Cu3Au-type structure. The Hf and Pt atoms locate at the (0, 0, 0) and (0.5, 0.5, 0) sites, respectively. The PtHf intermetallic compound is shown in Fig. 1. The Birch-Murnaghan (BM) equation of state (EOS) expressed as [9]:

\[ E(V) = E_0 + \frac{9V_0B_0}{16} \left( \left( \frac{V}{V_0} \right)^{7/3} - 1 \right) + B_0' \left( \left( \frac{V}{V_0} \right)^{5/3} - 1 \right) + 4 \left( \frac{V}{V_0} \right)^{2/3} \]  

(1)

Where \( V_0 \) represent equilibrium volume, \( E_0 \) represent total energy, \( B_0 \) represent equilibrium bulk modulus, and \( B_0' \) represent pressure derivative.

Figure 2 show the relationship between total energy and volume change of PtHf intermetallic compounds. Obviously, the equilibrium volume at the lowest energy is 65.13 (Å³). The Table 1 shown the equilibrium lattice parameters \( a \) (Å), equilibrium volume \( V \) (Å³), bulk modulus \( B_0 \) (GPa), its pressure...
derivative $B'$ and density $\rho$ (g/cm$^3$) of Pt$_3$Hf intermetallic compound. The present results are good consistent with the available experimental data [10] and the reference theoretical calculations results [11], which improve the data is reliable. The calculated density $\rho$ is about 0.8% lower than the result in Ref [12]. The lattice parameters ratios $a/a_0$ and lattice volume ratios $V/V_0$ as functions of pressure in the range from 0 to 100 GPa are shown in Fig. 3, explicit that the $a/a_0$ and $V/V_0$ decrease gradually with the increase pressure.

![Fig. 1. The crystal structure of L1$_2$ Pt$_3$Hf. The light gray atoms represent Pt, and the red atoms are Hf.](image)

![Fig. 2. The E-V data and EOS fitting curve of Pt$_3$Hf.](image)

**Table 1.** The equilibrium lattice parameters $a$ (Å), equilibrium volume $V$ (Å$^3$), density $\rho$ (g/cm$^3$), bulk modulus $B$ (GPa), and its pressure derivative $B'$ of Pt$_3$Hf calculated at zero pressure, compared with available experimental and theoretical results from references.

| Alloy   | $a$ [Å] | $V$ [Å$^3$] | $B_0$ [GPa] | $B'_0$ | $\rho$ [g/cm$^3$] |
|---------|---------|-------------|-------------|--------|-------------------|
| Pt$_3$Hf | This work | 4.023 | 65.13 | 236.99 | 4.9 | 19.470 |
|         | Exp     | 4.020 $^a$ | | | |
|         | Cals    | 4.029 $^b$ | | 238 $^c$ | | 19.626 $^d$ |

$^a$[13], $^b$[11], $^c$[14], $^d$[12]
Fig. 3. The variation of the lattice parameter ratio \( a/a_0 \) and the lattice volume ratio \( V/V_0 \) of Pt₃Hf compound with increasing pressure

3.2 Elastic properties

The elastic constants make great important parameters to reflecting the relation between stress and strain in a crystal. It is used to describe the mechanical crystals, dynamic and thermodynamic properties. There are three independent elastic constants used to describe the structure of cubic crystal system (\( C_{11}, C_{12} \) and \( C_{44} \)) [15]. The bulk modulus and shear modulus of Pt₃Hf intermetallic compound are calculated by using the Voigt-Reuss-Hill (VRH) approximation [16]. The calculation criteria are defined as [17]:

\[
B = \frac{(C_{11} + 2C_{12})}{3} \tag{2}
\]

\[
G_V = \frac{(C_{11} - C_{12} + 3C_{44})}{5} \tag{3}
\]

\[
G_R = 5(C_{11} - C_{12})C_{44} [4C_{44} + 3(C_{11} - C_{12})] \tag{4}
\]

\[
G = \frac{(G_V + G_R)}{2} \tag{5}
\]

\[
E = \frac{9GB}{3B + G} \tag{6}
\]

The calculated elastic constants and elastic modulus, \( B/G \) ratio, Poisson's ratio (\( \nu \)) and anisotropy index (\( A^2 \)) are shown in Table 2. Obviously, the values are good consistent with available theoretical data at zero pressure. The calculated elastic constants satisfy the mechanical stability criterion of cubic crystal \( C_{11} > 0, C_{44} > 0, C_{11} - C_{12} > 0, C_{11} + 2C_{12} > 0 \) under different pressures [18], indicating that Pt₃Hf intermetallic compound is satisfy mechanical stability within the scope of 0 to 100 GPa.

Table 2. The calculated elastic constants and elastic modulus, \( B/G \) ratio, Poisson's ratio (\( \nu \)) and anisotropy index (\( A^2 \)) of Pt₃Hf under different pressure (in GPa).

| \( p \) | \( C_{11} \) | \( C_{12} \) | \( C_{44} \) | \( B \) | \( G \) | \( E \) | \( P \) | \( B/G \) | \( A^2 \) |
|-------|---------|---------|---------|-------|-------|-------|----|-------|-------|
| Pt₃Hf |         |         |         |       |       |       |     |       |       |
| 0     | 351     | 181     | 126     | 238   | 120   | 309   | 0.280 | 1.98  |
| 0     | 353     | 178     | 129     | 236   | 110   | 287   | 0.298 | 2.13  | 1.48  |
| 10    | 403     | 206     | 153     | 272   | 128   | 333   | 0.296 | 2.11  | 1.56  |
| 20    | 450     | 232     | 176     | 305   | 145   | 377   | 0.294 | 2.09  | 1.61  |
| 30    | 496     | 261     | 197     | 340   | 160   | 416   | 0.296 | 2.11  | 1.68  |
| 40    | 542     | 291     | 219     | 374   | 175   | 454   | 0.298 | 2.13  | 1.74  |
| 50    | 583     | 318     | 238     | 406   | 188   | 490   | 0.299 | 2.15  | 1.79  |
The bulk modulus $B$ measures the resistance to volume changes. The shear modulus $G$ measures the resistance to shape change. The Young's modulus $E$ defined the stiffness of the material. The larger the result of Young's modulus $E$, the harder is the material. As shown the figure 4 shows the calculated elastic modulus of Pt$_3$Hf intermetallic compound under pressure, the bulk modulus $B$ shear modulus $G$ Young’s modulus $E$ increase linearly with the increase the pressure. Thus, the addition pressure contributes to an increase hardness and stiffness of the Pt$_3$Hf intermetallic compound.

![Graph](image)

**Fig. 4.** The calculated the elastic modulus of Pt$_3$Hf intermetallic compound with the different pressures.

The research of the mechanical properties of materials usually considers the effects of micro cracks and lattice distortion on its mechanical properties and the elastic anisotropy of elastic properties is usually a necessary condition for the two. Therefore, it is necessary to study the elastic anisotropy to improve the mechanical durability of the material. Figure 5, the calculated 3D Young’s modulus graph with the different pressure. For cubic structure Pt$_3$Hf, the Young’s modulus $E$ calculation criteria are defined as [19]:

$$\frac{1}{E} = S_{11}^{-2}(S_{11}^{-1} - S_{12}^{-1}) \frac{S_{44}}{2} (l_1^2 l_2^2 + l_2^2 l_3^2 + l_1^2 l_3^2)$$  \hspace{1cm} (7)

The $l_1$, $l_2$ and $l_3$ represents the direction cosines in the sphere coordination, $S_{ij}$ represent the elastic compliance constant. It can be obtained from the inverse of the elastic constant matrix. As is shown the Fig. 5, the Pt$_3$Hf intermetallic compound three-dimensional stereograms of Young’s modulus increase with the increasing pressure, which means higher pressure can improve the elastic anisotropy values and good to the hardness of the Pt$_3$Hf intermetallic compound.
Elastic anisotropy play an important role in physical and mechanical properties of material [20]. The anisotropy factor \(A^z\) measures the degree of anisotropy of the materials. If the \(A^z\) value equal to one, means the material completely isotropic. While the value departed from the value of one, means the elastic anisotropy of this material. From Table 2 and Fig. 6 (a), obviously that the all results of \(A^z\) no equal to one and larger than one and increase with increasing the pressure for Pt₃Hf intermetallic compound, which means that elastic anisotropy can be improved.

\[
A^z = \frac{2C_{44}}{C_{11} - C_{12}} \tag{8}
\]

It is well known that Poisson's ratio \(v\) \((-1 < v < 0.5)\) is used to measure the material's ability to resistance shear. The larger the value of Poisson's ratio, the stronger the resistance to shearing, the better the plasticity of the material [21]. If the value of \(v\) is less than 0.26, indicate the material it a brittle manner. Form Fig. 6 (b), it can observe all the Poisson’s ratio values of Pt₃Hf intermetallic compound are larger than 0.26 and increase with the pressure increases, it indicates that the increase in pressure can improve the plasticity.

\[
v = \frac{(E - 2G)}{2} \tag{9}
\]

Pugh [22] proposes the value of the ratio of \(B/G\) to judge the plasticity and brittleness of the material behaviors. The larger value of the \(B/G\) ratio related to the ductility, otherwise the low \(B/G\) ratio value related to brittleness. If \(B/G > 1.75\), the material behavior in a ductile nature, otherwise the material behavior in a brittle manner. As it can see form the Fig. 6 (c), the \(B/G\) ratio values performed an upward trend with raise the pressure, and the \(B/G\) ratio all values larger than 1.75, which indicates that Pt₃Hf intermetallic compound has a good ductility at higher pressures.

\[
B/G = 1.6 \tag{10}
\]
with the increase of pressures.

3.3 Debye temperature

The Debye temperature is a crucial role parameter describing the material. To further understand the thermodynamic properties and lattice stability under pressure, it is meaningful to calculate the $\Theta_D$ values at different pressures. We calculate the Deby temperatures for Pt$_3$Hf intermetallic compound calculated by using the average sound velocity and given by reference [23]:

$$\Theta_D = \frac{k_B}{\hbar} \left[ \frac{3n}{4k} \left( \frac{\rho N_A}{M} \right)^{1/3} \right] v_m$$

(10)

Where $h$ is the Planck’s constant, $k_B$ is the Boltzmann’s constant, $N_A$ is the Avogadro number, $\rho$ is the mass density of the material, $M$ is the molecular weight, $n$ is the number of atoms per formula unit. And the average elastic wave velocity $V_m$ is given by the equation:

$$V_m = \left( \frac{1}{3} \left( \frac{2}{v_l^3} + \frac{1}{v_t^3} \right) \right)^{-1/3}$$

(11)

Where $V_l$ and $V_t$ are longitudinal and transverse elastic sound velocities, respectively, which given by Navier’s equations [24].

$$v_l = \sqrt{\frac{B + 4G}{\rho}}$$

(12)

$$v_t = \sqrt{\frac{G}{\rho}}$$

(13)

Form the table 3, Fig. 7 and Table. 3 display the pressure dependence of longitudinal ($v_l$), transverse ($v_t$), average sound velocities ($v_m$), and Debye temperature ($\Theta_D$) of Pt$_3$Hf intermetallic compound increasing at the pressure increase. As the pressure increases, the covalent bond between the Hf atom and the Pt atom of the Pt$_3$Hf intermetallic compound increases. The present calculated results could be provided an effective prediction for the future experiment.

Table 3. The calculated longitudinal ($v_l$), transverse ($v_t$), average sound velocities ($v_m$) (m/s) and Debye temperature $\Theta_D$ (K) of Pt$_3$Hf compound with different pressure $P$ (GPa).

| Alloy  | $P$ (GPa) | $v_l$  | $v_t$  | $v_m$  | $\Theta_D$ |
|--------|-----------|--------|--------|--------|------------|
| Pt$_3$Hf | 0         | 4445.58| 2386.23| 2664.57| 312.99     |
|        | 10        | 4684.58| 2522.53| 2816.12| 335.01     |
|        | 20        | 4888.30| 2640.17| 2946.81| 354.42     |
|        | 30        | 5077.73| 2733.25| 3051.45| 370.46     |
|        | 40        | 5251.98| 2818.43| 3147.24| 385.41     |
|        | 50        | 5402.37| 2891.86| 3229.81| 398.43     |
|        | 60        | 5547.54| 2956.97| 3303.52| 410.31     |
|        | 70        | 5685.32| 3018.98| 3373.69| 421.75     |
|        | 80        | 5809.34| 3075.53| 3437.61| 432.21     |
|        | 90        | 5925.78| 3132.82| 3501.98| 442.82     |
|        | 100       | 6026.24| 3182.57| 3557.85| 452.26     |
Fig. 7. The calculated the $v_m$ (m/s) (a), $v_l$ (m/s) (b) and $v_t$ (m/s) (c) of Pt$_3$Hf compound with the different pressure.

3.4. Electronic properties

Electronic density of states is used to understand the mechanical and thermodynamic properties of materials. In order to further understand the electronic structure and chemical bonding strength character of Pt$_3$Hf compound, the total density of states (TDOS) and the density of partial states (PDOS) are calculated by first-principles based on the density function theory. Form the Fig. 8, there is no energy gap near the Fermi level, so the Pt$_3$Hf intermetallic compound exhibits metallic properties. The main bonding peaks of Pt$_3$Hf is predominantly derived from the Pt-5d and Hf-5d states in energy range, and the energy region from -10.2 eV to 7.4 eV. Meanwhile, we find the pseudogap occurs above Fermi level, shown the covalent bonding in Pt$_3$Hf compound.

Fig. 8. The total density of states (TDOS) and partial density of states (PDOS) for Pt$_3$Hf at 0 GPa.

The charge density difference distribution directly reflects the physical image of charge distribution in the system. The redistribution of charge density caused by pressure can be clearly shown, so that it has a more intuitive understanding of the bonding characteristics between atoms. The charge density difference is calculated as:

$$\Delta \rho = \rho(\text{Pt}_3\text{Hf}) - \rho(\text{Pt}_3) - \rho(\text{Hf})$$ (14)

Where $\rho(\text{Pt}_3\text{Hf})$, $\rho(\text{Pt}_3)$ and $\rho(\text{Hf})$ are the charge densities for the corresponding species with the same atoms coordinate. The charge density difference distribution is visualized by VESTA [25]. The effect of pressure on the charge density difference distribution has been investigated. From the Fig. 9, it is shown the
charge density difference in the (001) plane of Pt₃Hf at 0 GPa to 100 GPa. And we can know the lower density (blue) region higher density (red) region. And it is clear that with the pressure increase the charge is transfer Pt and Hf atoms and the covalent bonding between Pt and Pt is enhanced. The ionic bonding between Pt and Hf becomes stronger in pressure increase.

Fig. 9. Two-dimensional plane view of charge density difference distribution for Pt₃Hf intermetallic compound. The red color region indicates the positive charge density and blue one indicates the negative charge density.

4. Conclusions

To summarize, the structural, elastic, thermodynamic and electronic properties of Pt₃Hf compound under high pressure are studied by using the generalized approximation (GGA) calculations. The relevant conclusions are listed as follows:

(1) The calculated lattice parameter and volume are consistent with the experimental and theoretical results at zero pressure. The obtain elastic constant $C_{ij}$, bulk modulus $B$, shear modulus $G$, Young’s modulus $E$, $B/G$ ratio, Poisson’s ratio ($\nu$), are calculated. The results show that the mechanical more stable, has a high hardness and stiffness, ductility and plasticity all enhance under high pressure. The calculated anisotropic $A_Z$ and 3D curved surface of Young’s modulus relevant are all anisotropic at zero pressure and are more obviously anisotropic under high pressure.

(2) The Density of states (DOS) shows that the Pt₃Hf compound exhibits metallic characteristics. The difference charge density reveals the change of charge transfer under high pressure. It can conclude that the bonding strength between the atoms of the Pt₃Hf compound is enhanced under high pressure.

Acknowledgments

This work was financially supported by the National Natural Science Foundation of China (Nos. 51801179 and U1502272), the Yunnan Science and Technology Projects (Nos. 2018ZE001, 2018ZE006, 2018ZE016, 2018ZE021 and 2018ZE023), the Yunnan Applied Basic Research Projects (Nos. 2018FB083 and 2018FD011), the Yunnan Education Department Projects No. 2017ZZX232.

References
[1] L. A. Cornish, R. Süß, A. Watson, S. N. Prins, Building a Thermodynamic Database for Platinum-Based Superalloys: Part I. Platinum Metals Review 51, 104-115.

[2] Yanjun Liu, Huawei Huang, Yong Pan, Guanghui Zhao, Zheng Liang, First-principles study on the phase transition, elastic properties and electronic structure of Pt$_3$Al alloys under high pressure. Journal of Alloys and Compounds 597 (2014), 200-204.

[3] Xiao-Li Yuan, Mi-An Xue, Wen Chen, Tian-Qing An, Yan Cheng, Investigations on the structural, elastic and electronic properties of the orthorhombic Zirconium–Nickel alloy under different pressure. Computational Materials Science 65, 127-132.

[4] Adewumi Isaac Popoola, Lesley Heath Chown, Lesley Alison Cornish, Theoretical investigations of Pt$_3$X (X = Al, Sc, Hf, Zr) ground state. Turkish Journal of Physics 38 (2014), 10-16.

[5] P. J. Meschter, W. L. Metallurgical Transactions A Worrell, An investigation of high temperature thermodynamic properties in the Pt-Zr and Pt-Hf systems. 8 (1977), 503-509.

[6] Z. H. Sun, X. X. Wang, A. K. Soh, H. A. Wu, On stress calculations in atomistic simulations. Modell. Simul. Mater. Sci. Eng. 14 (2006), 423-431.

[7] J. Cormier, J. M. Rickman, T. J. Delph, Stress calculation in atomistic simulations of perfect and imperfect solids. J. Appl. Phys. 89 (2001), 99.

[8] J. P. Perdew, K. Burke, M. Ernzerhof, Generalized Gradient Approximation Made Simple. Physical Review Letters 77 (1998), 3865-3868.

[9] Francis Birch, Finite Elastic Strain of Cubic Crystals. Physical Review 71 (1947), 809-824.

[10] R. J. Wagner, L. Ma, F. Tavazza, L. E. Levine, Dislocation nucleation during nanoindentation of aluminum. Journal of Applied Physics 104 (2008), 601.

[11] Yuhua Zhang, Zhiyao Duan, Chan Xiao, Guofeng Wang, Density functional theory calculation of platinum surface segregation energy in Pt$_3$Ni (111) surface doped with a third transition metal. Surf. Sci. 605 (2011), 1577-1582.

[12] Weiwei Xing, Xing-Qiu Chen, Dianzhong Li, Yiyi Li, C. L. Fu, S. V. Meschel, Xueyong Ding, First-principles studies of structural stabilities and enthalpies of formation of refractory intermetallics: TM and TM3 (T=Ti, Zr, Hf; M=Ru, Rh, Pd, Os, Ir, Pt). Intermetallics 28 (2012), 16-24.

[13] L. M. Pecora, P. J. Ficalora, Some bulk and thin film properties of ZrPt3 and HfPt3. Journal of Electronic Materials 6 (1977), 531-540.

[14] ADEWUMI ISAAC POPOOLA, COMPUTATIONAL STUDY OF NOBLE METAL ALLOYS. (2013), pp. 143-156.

[15] J. Wang, S. Yip, S. R. Phillpot, D. Wolf, Crystal instabilities at finite strain. Phys Rev Lett 71 (1993), 4182-4185.

[16] V. Paidar, Yi-Shen Lin, M. Cak, V. Vitek, Why is the slip direction in CuZn and FeAl different than in CoTi? Intermetallics 18 (2010), 1285-1287.

[17] Liu Na, Xueye Wang, Yali Materials Chemistry Wan, Physics, First principles calculations of structural, elastic, electronic properties of Ir 3 Zr with L1 2 structure under high pressure. 162 (2015), 807-812.

[18] Dongmin Shi, Bin Wen, Roderick Melnik, Shan Yao, Tingju Li, First-principles studies of Al–Ni intermetallic compounds. Journal of Solid State Chemistry 182 (2009), 2664-2669.

[19] Jinghan Wang, Sidney Yip, S. R. Phillpot, Dieter Wolf, Crystal instabilities at finite strain.
Physical Review Letters 71, 4182-4185.

[20] Martin Ostoja-Starzewski, Luis Costa, Shivakumar I. Ranganathan, Scale-Dependent Homogenization of Random Hyperbolic Thermoelastic Solids. Journal of Elasticity 118 (2014), 243-250.

[21] B. Mayer, H. Anton, E. Bott, M. Methfessel, J. Sticht, J. Harris, P. Schmidt, Intermetallics 11 (2003) 23e32.,

[22] S. F. Pugh, XCII. Relations between the elastic moduli and the plastic properties of polycrystalline pure metals. The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science 45 (2009), 823-843.

[23] Orson L. Anderson, A Simplified Method for Calculating the Debye Temperature From Elastic Constants. Journal of Physics & Chemistry of Solids 24 (1963), 909-917.

[24] P Wachter, M Filzmoser, Rebizant Jean, Electronic and Elastic Properties of the Light Actinides Tellurides. 293 (2001), 199-223.

[25] K Momma, F Izumi, VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data. Journal of Applied Crystallography 44 (2011), 1272-1276.