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Study of the Physical and Mechanical Properties of Titanium in Volume by the MEAM Method

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Abstract

In this work we present the results of our study on the physical and mechanical properties of titanium in volume. The work consisted in determining its physical and mechanical properties under different crystallographic structures (HCP, FCC, BCC and SC) using the Modified Embedded Atom Method (MEAM) and the MEAM potential of titanium. We used the LAMMPS calculation code, based on classical molecular dynamics, to determine the most stable structure of titanium, which is the hexagonal compact structure (HCP) with crystal parameters a = 2.952 Å and c = 4.821 Å and a cohesion energy of −4.87 eV. This structure is seconded by the cubic centred structure (BCC) with a lattice parameter a = 3.274 Å and a cohesive energy of −4.84 eV. It was shown that titanium can crystallise into a third structure which is the face-centred cubic (FCC) structure with a lattice parameter a = 4.143 Å and a cohesive energy of −4.82 eV. The results obtained in this study were compared with the theoretical results and showed considerable agreement.

Keywords

MEAM Potential, LAMMPS Code, Molecular Dynamics, Elastic Constants, Modules, Ovito

1. Introduction

Titanium is a material whose market is perceived quite differently from other industrial materials. Its use implies high technology, purity, rarity, quality and unequalled strength. It represents 0.6% of the earth's crust and is ranked 4th

among the most abundant metals after iron, aluminum and magnesium [1].

Titanium as a chemical element has been known for more than 200 years, but it is only since 1920 that its real properties were discovered by Van Arckel and De Boer [2].

It was in 1791 that William Gregor, a British reverend, mineralogist and chemist discovered titanium. While examining the sand of the Helford River in the Menachan Valley in Cornwall, he isolated what he called black sand, now known as ilmenite [3] [4].

Professor Nsongo Timothée studied the structure and adhesion of thin films of titanium and titanium nitride prepared by sputtering [5]. In this study, he investigated the growth and structure of titanium and titanium nitride layers prepared on molybdenum, copper and tantalum by radio frequency magnetron and direct current triode sputtering. He also characterised the adhesion of titanium and titanium nitride to the different substrates used by the "scratch" method in order to relate the growth conditions and the resulting structural characteristics to the adhesion.

Stéphane GROSSO worked on Ti, TiN and TiOx architectural coatings developed by sputtering on stainless steel wires [6]. The main objective of his thesis was to understand the effects of the architecture of the coatings and of the processing parameters on the physicochemical characteristics of the Ti, TiN and TiO coatings and thus on their properties of use.

Abel Dominique EBOUNGABEKA, under the direction of Professor Timothée NSONGO, recently conducted a study on the reactivity of titanium dental implants in a salivary environment in the presence of food consumed in the Republic of Congo [7].

The aim of this work is to carry out a study of the physical and mechanical properties of titanium using the MEAM method, under the LAMMPS code, in order to determine its most stable crystal structure.

2. Methodology

We ran a simulation under the LAMMPS code version 2020 with the executable lmp_mpi, under the Windows operating system, using the MEAM potentials found in the database at https://www.ctcms.nist.gov/potentials/system (**Table 1**).

The MEAM potential of Titanium used in this work was developed by Y.-M. Kim, B.-J. Lee, and M.I. Baskes (2006), and its parameters are aligned in the following table [8].

This potential was used to calculate the cohesive energies under different crystallographic structures using the MPCV4 application.

The calculations were simulated for periodic crystallographic structures for 2 × 2 × 2 mesh under Lamps (**Figure 1**).

3. Results and Discussion

In the following paragraphs we present the results obtained under the LAMMPS

Table 1. Titanium potential and screening parameters.

(a)

elt	atwt	alat	β_0	β_1	β_2	β_3	t_0	t_1	t_2	t_3	esub	asub	α	Z	lat	ibar	rozero
Ti	47.88	2.92	2.7	1.0	3.0	1.0	1.0	6.8	−2.0	−12.0	4.87	0.66	4.71	12	*hcp*	*3.0*	*1.0*

(b)

delr	0.1
augt1	0
erose_form	2
ialloy	2
zbl(1,1)	0
nn2(1,1)	1
rho(0,1)	1.000
Ec(1, 1)	4.870
re(1, 1)	2.9200
alpha(1, 1)	4.71945
repuls(1, 1)	0.00
attrac(1, 1)	0.00
Cmin(1, 1, 1)	1.00
Cmax(1, 1, 1)	1.44

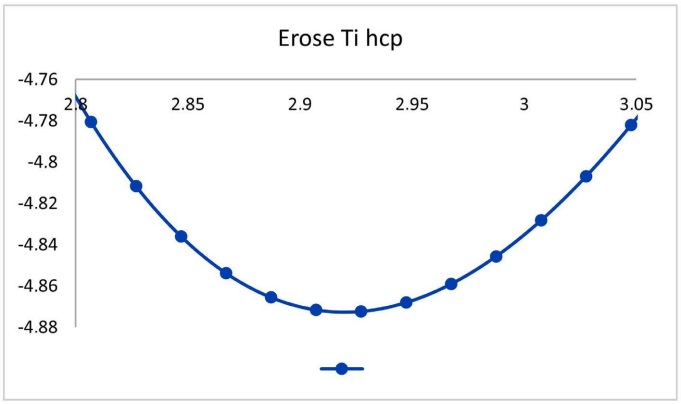

Figure 1. Rose energy of titanium in HCP structure.

code using the MEAM potentials, these results were also calculated by the MPCV4 application under Windows 10, 64 bits.

The crystalline parameters, elastic constants and structural stability moduli for different titanium structures are presented.

3.1. Crystalline Parameters

The presented crystal parameters and volumes have been calculated for HCP, CFC, BCC, SC structures and are presented in **Table 2**.

Table 2. Crystal parameters by structure and crystallographic volume.

Structures	a (Å)	b (Å)	c (Å)	Volumes (Å)^3
HCP	2.952	2.952	4.821	35.215
FCC	4.143	4.143	4.143	17.649
BCC	3.274	3.274	3.274	34.842
SC	2.780	2.780	2.780	21.332

The most voluminous structure is the HCP structure followed by the BCC structure, SC and finally the FCC structure.

3.2. Cohesive Energy

The MEAM potential of Titanium has allowed us, thanks to the MPCV4 application, to represent the cohesion energies for different structures as shown in **Figure 2** and **Figure 3**.

We also calculated the cohesion energies in different crystallographic structures for titanium; we realised that the HCP structure of the Ti type is the most stable with a cohesion energy of −4.87 eV followed by the BCC structure with a cohesion energy of −4.84 eV (**Table 3**).

The evolution of the cohesion energy per structure is shown in **Figure 4** and **Figure 5**.

Although the number of atoms per cell increases in some structures, the cohesive energy becomes very large, reflecting the instability of the structure; the HCP and FCC structures are very similar.

3.3. Mechanical Properties

For the temperature of 298 Kelvin, we calculated the elastic constants of titanium in the hexagonal phase and the corresponding elastic moduli.

3.3.1. Elastic Constants

Elastic constants C_{ij} are essential parameters for predicting the physical properties and mechanical stability of materials [9] [10].

For elements with a cubic structure, the criterion for predicting structural stability is as follows [11] [12]:

$$C_{11}-C_{12}>0,\ C_{11}>0,\ C_{44}>0,\ C_{11}+2C_{12}>0 \tag{1}$$

For elements that have a tetragonal structure, we have this [13] [14]:

$$C_{11}>\left|C_{12}\right|,\ C_{44}>0,\ C_{66}>0,\ C_{33}\left(C_{11}+C_{12}\right)>2C_{13}^2 \tag{2}$$

And for elements with a hexagonal structure, we have [15] [16]:

$$C_{44}>0,\ C_{11}-C_{12}>0,\ C_{33}\left(C_{11}+C_{12}\right)>2C_{13}^2 \tag{3}$$

However, the matrix linking the deformations and the elastic constants is represented by the following relation.

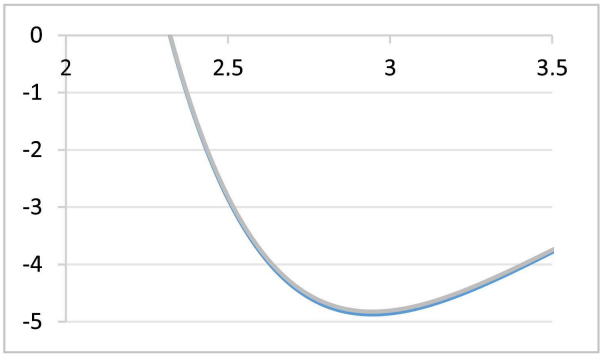

Figure 2. Cohesive energies of titanium in HCP and FCC.

Figure 3. Cohesive energies of BCC and SC titanium.

Table 3. Cohesive energy per structure.

Structures	Parameters (Å)	Total energy (eV)	Ecoh (eV)	Number of atoms
FCC	4.14	−19.29	−4.82	4
HCP	2.95	−19.48	−4.87	4 (more stable)
BCC	3.27	−9.69	−4.84	2
SC	2.78	−3.62	−3.62	1

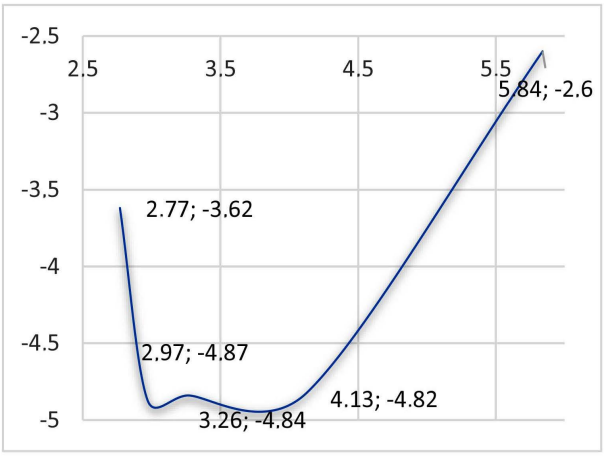

Figure 4. Cohesion energy by crystal structure.

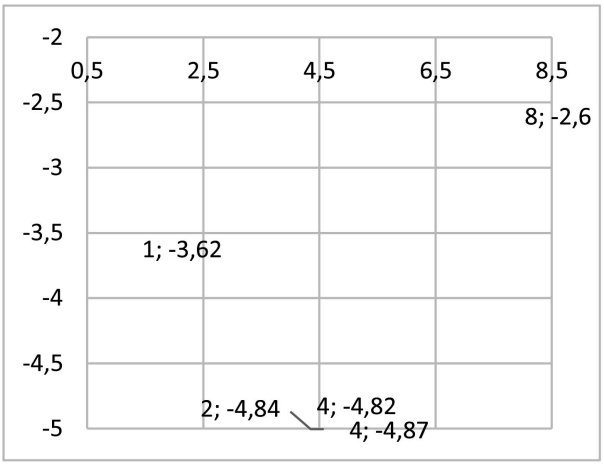

Figure 5. Cohesive energy per atom number.

$$\begin{pmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\\ \sigma_4\end{pmatrix}=\begin{pmatrix}C_{11} & C_{12} & C_{13} & C_{14}\\ C_{21} & C_{22} & C_{23} & C_{24}\\ C_{31} & C_{32} & C_{33} & C_{34}\\ C_{41} & C_{42} & C_{43} & C_{44}\end{pmatrix}\begin{pmatrix}\varepsilon_1\\ \varepsilon_2\\ \varepsilon_3\\ \varepsilon_4\end{pmatrix} \tag{4}$$

The elastic constants for the hexagonal structure of titanium have been calculated and are presented in **Table 4**.

The exploitation of these data allows us to compare the elastic constants between them and between the theoretical and experimental data through the **Figure 6** and **Figure 7**.

The order of magnitude is well defined by C33 > C11 > C12 > C13 > C44 and is preserved in the theory as well as for experimental data.

3.3.2. Elastic Modules

In this section we present the elastic moduli according to the Voigt-Reuss-Hill scheme. These moduli reflect the stiffness and flexibility of the material against external excitations and they reflect the direction of the resulting deformation or the resulting stress. They are also referred to as elastic coefficients, which are simply the engineer's moduli for the properties of nanomaterials. We give here the mathematical relations between Young's modulus, Poisson's ratio and shear coefficient with the elastic constants [19] [20].

- The H-symbol stiffness is an important parameter for materials that can be estimated as the ability to resist localized deformation [21] [22]. Defects and grain size of materials are of great importance with regard to hardness. The hardness H is given by the following semi-empirical formula [23]:

$$H=\frac{(1-2v)}{6(1+v)}E \tag{5}$$

- The elastic moduli (Bulk modulus B, Shear modulus G and Young's modulus E) are estimated by the Voigt-Reuss-Hill method. Generally, the larger the B, the greater the resistance of the material to change in volume.

Table 4. Comparison of theoretical and experimental constants.

Elastic constants of the HCP reference structure (GPa)			
	Our work	Theory [17]	Exp.(298˚K) [18]
C11	170.046	171.600	176.100
C12	80.415	86.600	86.900
C13	74.7852	72.600	68.300
C33	187.088	190.600	190.500
C44	42.0824	41.100	50.800

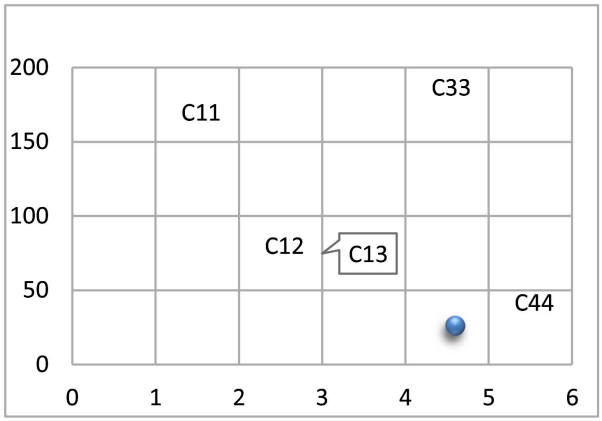

Figure 6. Elastic constants of titanium in point cloud.

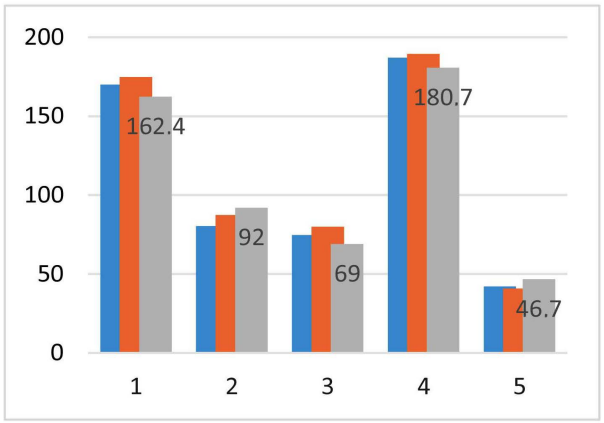

Figure 7. Values of Elastic constants in a histogram.

- The elastic anisotropy A^U plays a vital role in physical/mechanical processes such as fracture behavior and phase transformations [24]. It is given by the following formula [25]:

$$A = U5\frac{G_v}{G_R} + \frac{B_v}{B_R} - 6 \tag{6}$$

where G_v and G_R represent Voigt and Reuss' Shear modulus, B_v and $\frac{B_v}{B_R}$ are the Bulk modulus of Voigt and Reuss.

Table 5. Mathematical expressions of elastic moduli for a hexagonal structure [26] [27] [28].

$E=\frac{9BG}{3B+G}$	$v=\frac{(3B-2G)}{(6B+2G)}$	$B=\frac{C_{11}+2C_{12}}{3}$
$G=\frac{3c_{44}+c_{11}-c_{12}}{5}$	$C_{66}=\frac{C_{11}-C_{12}}{2}$	$M=C_{11}+C_{12}+2C_{33}-4C_{13}$
$B_{Hill}=\frac{1}{2}\left(B_{Reuss}+B_{Voigt}\right)$	$B_R=\frac{(C_{11}+C_{12})C_{33}-2C_{13}^2}{C_{11}+C_{12}-4C_{13}+2C_{33}}$	$B_V=\frac{2C_{11}+2C_{12}+4C_{13}+C_{33}}{9}$
$G_{Hill}=\frac{1}{2}\left(G_{Reuss}+G_{Voigt}\right)$	$G_R=\frac{5(C_{11}-C_{12})C_{44}}{4C_{44}+3(C_{11}-C_{12})}$	$G_v=\frac{C_{11}+C_{12}-4C_{13}+2C_{33}+12C_{44}+12C_{66}}{30}$

Table 6. Elastic modules.

Elastic modules (Gpa)						
Size	Symbols	Voigt	Reuss	Hill	Theory [29]	Exp, 298˚K [30]
Bulk modulus	B	109.68	109.59	109.64	110.82	109.96
Shear modulus	G	45.61	43.14	44.38	44.68	50.16
Young modulus	E		117.14		118.15	130.62
Hardness	H		5.257		-	-
Elastic anisotropy	A^U		0.287		-	-
Fish ratio	V		0.322		0.322	0.302

In the table below, we present all the elastic moduli in different systems of approaches for a crystallographic structure (Table 5).

The results obtained from the expressions of the previous modules are presented in Table 6.

It can be seen from this table that the elastic moduli calculated from the Lammps code using the MEAM potential is in good agreement with the theoretical and experimental results. Hence the MEAM potential used is an appropriate potential for the study of metals as it takes into account steric and angular effects in the system studied.

4. Conclusion

During this study on the physical and mechanical properties of titanium in volume using the Lammps calculation code and the MEAM potential, we studied this metal in the four different structures namely BCC (cubic centred), FCC (face centred cubic), HCP (hexagonal compact) and SC (simple cubic) in order to determine its most stable structure and its physical and mechanical properties. We found that the most stable structure is the compact hexagonal structure with a mesh parameter a = 2.97 Å, c = 4.821 Å and a cohesive energy Ecoh = −4.87 eV followed by the face-centred cubic (BCC) structure and then the face-centred cubic (FCC) structure which is a transient structure. Finally, we calculated the elastic constants and moduli of elasticity and it was found that our results are in accordance with the theoretical results and this proves sufficiently

the effectiveness of the MEAM potential used to carry out this study.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

References

[1] Lutjering, G. and Williams, J.C. (2003) Titanium. Springer, Berlin. https://doi.org/10.1007/978-3-540-71398-2

[2] Van Arkel, A.E. and de Boer, J.H. (1925) Darstellung von reinem Titanium-, Zirkonium-, Hafnium- und Thoriummetall. *Zeitschrift für anorganische und allgemeine Chemie*, **148**, 345-350. https://doi.org/10.1002/zaac.19251480133

[3] Leyens, C. and Peters, M. (2003) Titanium and Titanium Alloys, Fundamentals and applications. Wiley, New York. https://doi.org/10.1002/3527602119

[4] Combres, Y. (1999) Properties of Titanium and Its Alloys. Techniques de l'ingénieur M557.

[5] Nsongo, T. (1987) Study of the Structure and Adhesion of Titanium Nitride Thin Films Prepared by Sputtering. https://www.theses.fr/1987AIX30051

[6] Grosso, S. (2017) Architectural Coatings of Ti, TiN and TiOx Grown by Flow Sputtering on Stainless Steel Wires. https://www.theses.fr/2017GREAI083

[7] Eboungabeka, A.D., Trigo, E.R.M.E. and Nsongo, T. (2021) Reactivity of Titanium Dental Implants in Salivary Environment in the Presence of Foods Consumed in the Republic of the Congo. *Advances in Materials Physics and Chemistry*, **11**, 93-99. https://doi.org/10.4236/ampc.2021.115009

[8] Kim, Y.M., Lee, B.J. and Baskes, M.I. (2006) Modified Embedded-Atom Method Interatomic Potentials for Ti and Zr. *Physical Review B*, **74**, Article ID: 014101. https://doi.org/10.1103/PhysRevB.74.014101

[9] Wang, J.H., Lu, Y., Zhang, X.L. and Shao, X.H. (2018) The Elastic Behaviors and Theoretical Tensile Strength of γ-TiAl Alloy from the First Principles Calculations. *Intermetallics*, **101**, 1-7. https://doi.org/10.1016/j.intermet.2018.07.001

[10] Mouhat, F. and Coudert, F.X. (2014) Necessary and Sufficient Elastic Stability Conditions in Various Crystal Systems. *Physical Review B*, **90**, Article ID: 224104. https://doi.org/10.1103/PhysRevB.90.224104

[11] Tian, J., Zhao, Y., Wang, B., Hou, H. and Zhang, Y. (2018) The Structural, Mechanical and Thermodynamic Properties of Ti-B Compounds under the Influence of Temperature and Pressure: First-Principles Study. *Materials Chemistry and Physics*, **209**, 200-207. https://doi.org/10.1016/j.matchemphys.2018.01.067

[12] Xiao, B., Feng, J., Zhou, C.T., Jiang, Y.H. and Zhou, R. (2011) Mechanical Properties and Chemical Bonding Characteristics of Cr_7C_3 Type Multicomponent Carbides. *Journal of Applied Physics*, **109**, Article ID: 083521.

https://doi.org/10.1063/1.3532038

[13] Hu, H., Wu, X., Wang, R., Jia, Z., Li, W. and Liu, Q. (2016) Structural Stability, Mechanical Properties and Stacking Fault Energies of $TiAl_3$ Alloyed with Zn, Cu, Ag: First-Principles Study. *Journal of Alloys and Compounds*, **666**, 185-196. https://doi.org/10.1016/j.jallcom.2016.01.106

[14] Qi, Y.Y., Mu, Y., Cheng, Y. and Ji, G.F. (2015) Pressure Effect on Electronic, Elastic and Optical Properties of Eu: CaF_2 Crystal: A First-Principles Study. *Philosophical Magazine*, **95**, 2974-2989. https://doi.org/10.1080/14786435.2015.1082664

[15] Li, X.-H., Cui, H.-L. and Zhang, R.-Z. (2017) Theoretical Study on the Structural, Mechanical, Electronic Properties and QTAIM of CrB4 as a Hard Material. *Chinese Physics B*, **26**, Article 096201. https://doi.org/10.1088/1674-1056/26/9/096201

[16] Sinko, G.V. and Smirnow, N.A. (2002) *Ab initio* Calculations of Elastic Constants and Thermodynamic Properties of bcc, fcc, and hcp Al Crystals under Pressure. *Journal of Physics: Condensed Matter*, **14**, 6989-7005. https://doi.org/10.1088/0953-8984/14/29/301

[17] Ikehata, H., Nagasako, N., Furuta, T., Fukumoto, A., Miwa, K. and Saito, T. (2004) First-Principles Calculations for Development of Low Elastic Modulus Ti Alloys. *Physical Review B*, **70**, Article ID: 174113. https://doi.org/10.1103/PhysRevB.70.174113

[18] Simmons, G. and Wang, H. (1971) Single Crystal Elastic Constants and Calculated Aggregate Properties, A Handbook. MIT Press, Cambridge.

[19] Voigt, W. (1889) Ueber die Beziehung zwischen den beiden Elasticitätsconstanten isotroper Körper. *Annalen der Physik*, **274**, 573-587. https://doi.org/10.1002/andp.18892741206

[20] Hill, R. (1963) Elastic Properties of Reinforced Solids: Some Theoretical Principles. *Journal of the Mechanics and Physics of Solids*, **11**, 357-372. https://doi.org/10.1016/0022-5096(63)90036-X

[21] Gao, F.M. and Gao, L.H. (2010) Microscopic Models of Hardness. *Journal of Superhard Materials*, **32**, 148-166. https://doi.org/10.3103/S1063457610030020

[22] Chen, X.Q., Niu, H., Li, D. and Li, Y. (2011) Modeling Hardness of Polycrystalline Materials and Bulk Metallic Glasses. *Intermetallics*, **19**, 1275-1281. https://doi.org/10.1016/j.intermet.2011.03.026

[23] Yousef, E.S., El-Adawy, A. and El-Kheshkhany, N. (2006) Effect of Rare Earth (Pr_2O_3, Nd_2O_3, Sm_2O_3, Eu_2O_3, Gd_2O_3 and Er_2O_3) on the Acoustic Properties of Glass Belonging to Bismuth-Borate System. *Solid State Communications*, **139**, 108-113. https://doi.org/10.1016/j.ssc.2006.05.022

[24] Ledbetter, H. and Migliori, A. (2006) A General Elastic-Anisotropy Measure. *Journal of Applied Physics*, **100**, Article ID: 063516. https://doi.org/10.1063/1.2338835

[25] Ranganathan, S.I. and Ostoja-Starzewski, M. (2008) Universal Elastic Anisotropy Index. *Physical Review Letters*, **101**, Article ID: 055504. https://doi.org/10.1103/PhysRevLett.101.055504

[26] Wu, Z.J., Zhao, E.J., Xiang, H.P., Hao, X.F., Liu, X.J. and Meng, J. (2007) Crystal Structures and Elastic Properties of Superhard IrN2 and IrN_3 from First Principles. *Physical Review B*, **76**, Article ID: 054115. https://doi.org/10.1103/PhysRevB.76.059904

[27] Reuss, A. (1929) Berechnung der Fließgrenze von Mischkristallen auf Grund der Plastizitätsbedingung für Einkristalle. *Zeitschrift für Angewandte Mathematik und*

Mechanik, **9**, 49-58. (In German) https://doi.org/10.1002/zamm.19290090104

[28] Voigt, W. (1928) Lehrbuch der Kristallphysik. Taubner, Leipzig.

[29] Li, H., Chen, Y., Wang, H., Wang, H., Li, Y., Harran, I., *et al.* (2017) First-Principles Study of Mechanical and Thermodynamic Properties of Ti-Ga Intermetallic Compounds. *Journal of Alloys and Compounds*, **700**, 208-214. https://doi.org/10.1016/j.jallcom.2017.01.052

[30] Jiang, D.Y., Ouyang, C.Y. and Liu, S.Q. (2016) Mechanical Properties of W-Ti Alloys from First-Principles Calculations. *Fusion Engineering and Design*, **106**, 34-39. https://doi.org/10.1016/j.fusengdes.2016.03.028