Elastic properties and Debye Temperature of Tetragonal and Cubic Ga₃Zr Under High Pressure: A First-Principles Investigation

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Keywords: Density functional theory calculations; Elastic properties; High pressure

Abstract. Two different phases of Ga₃Zr with tetragonal ($D0_{22}$) and cubic ($L1_2$) structures under high pressure are investigated by using density functional theory (DFT) calculations. The elastic constants (C_{ij}) and mechanical moduli, including bulk modulus (B) and shear modulus (G), are calculated under various pressures. When pressure goes up, the increasing tendency of C_{ij} , B and Gare confirmed. On the basis of Pugh's criterion, $L1_2$ -Ga₃Zr has better ductility comparing with $D0_{22}$ -Ga₃Zr under various pressures in the range of 0~60 GPa. The brittleness of $D0_{22}$ -Ga₃Zr depends on the pressure, it will become ductile when the pressure rise up higher than ~35 GPa. For the both phases, Debye temperature (Θ_D) is also calculated under high pressures. For the both phases, Debye temperature increases with pressure rising up. Under pressures ranging from 0 GPa to 60 GPa, the Θ_D values of $L1_2$ -Ga₃Zr are lower than the ones of $D0_{22}$ -Ga₃Zr.

Introduction

The properties of materials are usually related to their circumstances. Besides the factor of temperature, pressure also significant influences the properties of materials. In recent years, by using density functional theory (DFT) calculation method, the theoretical studies about materials' properties under high pressure have been commonly conducted. For example, the elastic properties of MgSiO₃ under lower mantle conditions were investigated by first principle calculations [1], which is on the basis of DFT. The pressure-induced effects on the elastic and mechanical properties of TiC and TiN were also studied by using DFT calculations [2].

The DFT calculations are also performed to investigate Ga-Zr intermetallics. For Ga₃Zr and Ga₂Zr, the crystallochemical affinity and optical functions[3], and their band structure, density of states, and crystal chemistry[4] were studied by using all-electron full potential linearized augmented plane wave (FP-LAPW) method. Furthermore, the phase equilibriums of Ga–Zr system were investigated by combining experimental investigation and thermodynamic modeling, the formation enthalpies phases of Ga-Zr intermetallics (including Ga₃Zr, Ga₂Zr, etc.) were computed via first-principles calculations, and the calculated phase diagram and thermodynamic properties agreed well with the available experimental data [5].

However, according to our knowledge, the pressure's influence on the elastic and mechanical properties of Ga₃Zr is rarely reported. Under normal temperature and pressure, the compound Ga₃Zr exhibit tetragonal structure ($D0_{22}$, I4/mmm) [5, 6], and the cubic structure ($L1_2$, $Pm\bar{3}m$) is a metastable phase. It is natural to question that, the elastic and mechanical properties of Ga₃Zr may vastly change under high pressure. The present work is conducted to clarify the dependence of elastic and mechanical properties of $D0_{22}$ - and $L1_2$ -Ga₃Zr under various pressures from 0 GPa to 60 GPa.

Computational methodology

The DFT calculations in present work were conducted using CASTEP package [7, 8], and plane-wave ultrasoft pseudopotentials [9, 10] were employed. The valence electrons considered in the pseudopotentials were Ga $3d^{10}4s^24p^1$, Zr $4s^24p^64d^25s^2$, respectively. The exchange correlation (XC) energy was treated with two different forms: generalized gradient approximation (GGA) functionals of PBE [11], and local density approximation (LDA) functional of CAPZ [12, 13]. The convergence threshold in the self consistent field (SCF) procedure was set as 5.0×10^{-7} eV/atom. In the minimization with Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm, the convergence tolerances for the energy, force, stress and displacement were set as 5.0×10^{-6} eV/atom, 0.01 eV/Å, 0.02 GPa and 5×10^{-4} Å, respectively. After the validation of convergence tests, the cutoff energy on the plane wave basis was set as 350 eV, the *k*-points grids were set as $20 \times 12 \times 20$, $40 \times 40 \times 22$, $24 \times 24 \times 24$ and $24 \times 24 \times 10$ for bulk α -Ga (A11, Cmca)[14], hcp-Zr (A3, P6_3/mmc)[15], L1₂- and $D0_{22}$ -Ga₃Zr respectively. The above *k*-points settings make the separation of the reciprocal space around 0.01Å⁻¹.

After fully optimizations, the calculated equilibrium lattice constants and previous experimental data are listed in Table 1, the elastic constants (C_{ij}) and formation energy ΔE_f (Ga₃Zr) are listed in Table 2. For the both XC potentials, the calculated lattice constants agree well with the available experimental data, their deviations are in the ranges of $-1.4\% \sim 5.1\%$ and $-3.8\% \sim 2.6\%$ for GGA-PBE and LDA-CAPZ potentials, respectively. For $D0_{22}$ -Ga₃Zr, our calculated lattice parameters with GGA-PBE potential are very close to previous results (a = 3.9875 Å, c = 8.7961 Å) in other DFT literature [5]. Besides that, our calculated formation energy $\Delta E_f(D0_{22}$ -Ga₃Zr) is also accordance with the previous calculation [5]. Therefore, the calculation parameters adopted in our work are validated, and the calculations accuracy is adequate.

Moreover, the "over-binding effect" of LDA potential reported in other calculations [16-20] is also shown in our calculations, the lattice constants calculated with LDA-CAPZ potential is slightly smaller that the results of GGA-PBE potential.

Dhaga	Space	Pearson	Strukturbericht	Lattice parameters (Å)			
Phase	group (#)	symbol	designation	Present Calc.	Expt.		
α-Ga	<i>Cmca</i> (64)	<i>oC</i> 8	A11	a=4.5776, b=7.7406, $c=4.5727^{a}$	<i>a</i> =4.519, <i>b</i> =7.658, <i>c</i> =4.526[14]		
				a=4.4177, b=7.4829, c=4.4271 ^b			
hcp-Zr	P6 ₃ /mmc (194)	hP2	A3	<i>a</i> =3.2298, <i>c</i> =5.1711 ^a	<i>a</i> =3.2331, <i>c</i> =5.1480[15]		
				$a=3.1468, c=5.0793^{b}$			
$D0_{22}$ -Ga ₃ Zr	I4/mmm (139)	<i>t1</i> 8	<i>D</i> 0 ₂₂	<i>a</i> =3.9160, <i>c</i> =9.1713 ^a	<i>a</i> =3.963, <i>c</i> =8.730[5]		
				<i>a</i> =3.8220, <i>c</i> =8.9522 ^b	a=3.971,c=8.729[6]		
$L1_2$ -Ga ₃ Zr	$Pm\overline{3}m$	cP4	$L1_2$	<i>a</i> =4.1245 ^a			
	(221)			<i>a</i> =4.0218 ^b			

Table 1	Crystallographi	c data, lattice	constants of l	bulk Ga,	Zr and Ga ₃ Zr.
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Note: Superscripts "a" and "b" denote the results calculated with exchange correlation functionals of GGA-PBE and LDA-CAPZ, respectively.

Dhagag	Data source	Elastic	$\Delta E_f(\text{Ga}_3\text{Zr})$						
Phases		C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	B_0	(kJ/mol)
$D0_{22}$ -Ga ₃ Zr	Present calculation with GGA-PBE	181.16	85.14	47.26	180.68	75.79	113.76	99.89	-46.304
	Present calculation with LDA-CAPZ	219.37	105.39	59.36	215.49	88.98	135.32	121.96	-52.606
	Other calculation with GGA-PBE in Ref. [5]								-53.727 °
L1 ₂ - Ga ₃ Zr	Present calculation with GGA-PBE	133.30	78.06			42.06		96.47	-43.923
	Present calculation with LDA-CAPZ	149.19	95.33			50.32		113.28	-50.433

Table 2 Elastic constants (C_{ij}) and formation energy (ΔE_f) of $L1_2$ - and $D0_{22}$ -Ga₃Zr.

Note: ^a An approximate value of first-principle calculation with GGA-PBE potential under 0 GPa in Ref. [5].

Results and Discussion

Elastic Constants. The elastic constants of solids can be used to calculate their mechanical and thermodynamic properties. Commonly, the single crystal's elastic constants C_{ij} can be obtained by calculating the total energy as a function of appropriate strains [21-23]. To calculate the elastic constants, a serial of deformed cells (strain) are introduced and optimized to calculate the tensor of elastic constants. The elastic strain energy U of a deformed crystal cell is given as [24]:

$$U = \frac{\Delta E}{V_0} = \frac{1}{2} \sum_{ij} C_{ij} e_i e_j \tag{1}$$

where ΔE is the energy difference of deformed cell relative to the unstrained cell, V_0 is the volume of the equilibrium cell without any deformation, C_{ij} s are the elastic constants, e_i and e_j are strain.

For the L_{1_2} structure, there are three independent elastic constants: $C_{11}=C_{22}=C_{33}$, $C_{12}=C_{13}=C_{23}$, $C_{44}=C_{55}=C_{66}$; for the $D0_{22}$ structure, there are six independent constants: $C_{11}=C_{22}$, C_{12} , $C_{13}=C_{23}$, C_{33} , $C_{44}=C_{55}$, C_{66} . The obtained monocrystal quantities, such as these elastic constants, can not accurately stand for the properties of polycrystalline materials, so they should be further calculated and rectified. The polycrystalline mechanical quantities, such as bulk modulus (*B*), shear modulus (*G*), Young's modulus (*E*), Poisson's ratio (*v*), can be calculated from these independent elastic constants.

There are three different algorithms corresponding to different bound to calculate these polycrystalline mechanical quantities: the Voigt bound is obtained by the average polycrystalline modules based on an assumption of uniform strain throughout a polycrystal, and it is the upper limit of the actual effective modules; while the Reuss bound is obtained by assuming a uniform stress, and it is the lower limit of the actual effective modules; the arithmetic average of Voigt and Reuss bounds is termed as the Voigt-Reuss-Hill approximation. The formula for calculating these mechanical quantities can be given as follows: (1) for the cubic $L1_2$ structures, $B_V = B_R =$

 $(C_{11}+2C_{12})/3$, $G_{\rm V} = (C_{11}-C_{12}+3C_{44})/5$, $G_{\rm R} = 5(C_{11}-C_{12})C_{44}/[4C_{44}+3(C_{11}-C_{12})][25];$ (2) for the tetragonal $D0_{22}$ structures, $B_{\rm V} = (1/9)[2(C_{11}+C_{12})+C_{33}+4C_{13}]$, $B_{\rm R} = C^2/M$, $G_{\rm V} = (1/30)(M+3C_{11}-3C_{12}+12C_{44}+6C_{66})$, $G_{\rm R} = 15\{(18B_{\rm V}/C^2)+[6/(C_{11}-C_{12})]+(6/C_{44})+(3/C_{66})\}^{-1}$, $M = C_{11}+C_{12}+2C_{33}-4C_{13}$, $C^2 = (C_{11}+C_{12})C_{33}-2(C_{13})^2[26]$; and (3) for the Voigt-Reuss-Hill approximation, $B_{\rm H} = (1/2)(B_{\rm V} + B_{\rm R})$, $G_{\rm H} = (1/2)(G_{\rm V} + G_{\rm R})$, the subscript letter of V, R and H denote Voigt, Reuss bound and Hill approximation, respectively. The $B_{\rm H}$ and $G_{\rm H}$ are adopted in this paper to calculate Young's modulus *E* and Poisson's ratio *v* by the following formulas: E = 9BG/(3B+G), v = (3B-2G)/[2(3B+G)] [27].

The elastic constants of $D0_{22}$ - and $L1_2$ -Ga₃Zr under 0 Gpa are calculated with GGA-PBE and LDA-CAPZ functionals, the results are presented in Table 2. Due to the data of Ga₃Zr are rarely reported in other literatures, the comparison of elastic constants between our results and previous data is unavailable. However, the bulk modulus of Al₃Zr at 0 GPa was empirically predicted as B_0 =95.4 GPa[28], and the elastic constants of $L1_2$ -Al₃Zr were calculated as C_{11} =184.8 GPa, C_{12} =59.9 GPa, C_{44} =72.0 GPa, B_0 = 101.5GPa with GGA-PW91 potential[29]. Comparing with these elastic and mechanical data of Al₃Zr, our calculation results of Ga₃Zr are reasonable.

Moreover, the elastic constants under high pressures (5~60 GPa) are also calculated with GGA-PBE and LDA-CAPZ potentials, and the results are presented in Table 3. It is confirmed that the elastic constants and mechanical moduli increase with the pressure increasing, which indicates the materials will be stiffer and more difficult to be compressed under higher pressure.

Phases	XC	Pressure (GPa)	C_{11}	C_{12}	C_{13}	<i>C</i> ₃₃	C_{44}	C ₆₆	В	G	Ε	v	B/G
D0 ₂₂ -	GGA	0	181.16	85.14	47.26	180.68	75.79	113.76	99.89	74.47	178.93	0.20	1.34
Ga ₃ Zr		10	243.22	125.93	74.85	249.60	99.47	150.51	142.64	96.24	235.72	0.22	1.48
		20	291.45	164.27	104.49	307.84	120.03	182.46	181.60	112.60	279.94	0.24	1.61
		30	348.75	201.94	131.46	363.54	138.70	211.38	220.74	130.05	326.10	0.25	1.70
		40	393.63	241.88	158.80	419.49	155.78	238.15	257.98	143.41	362.97	0.27	1.80
		50	440.77	278.78	186.45	477.09	171.81	263.42	295.40	157.23	400.61	0.27	1.88
		60	483.77	312.47	210.87	524.41	186.81	287.27	328.52	169.80	434.52	0.28	1.93
	LDA	0	219.37	105.39	59.36	215.49	88.98	135.32	121.96	87.97	212.76	0.21	1.39
		10	277.84	143.65	86.96	233.02	111.48	170.66	156.08	104.94	257.18	0.23	1.49
		20	329.51	183.85	116.33	341.89	131.56	201.93	203.31	125.34	311.92	0.24	1.62
		30	379.69	222.48	145.14	397.12	149.61	230.33	241.96	140.52	353.19	0.26	1.72
		40	428.34	259.96	173.00	451.38	166.54	256.86	279.49	154.91	392.25	0.27	1.80
		50	475.23	296.46	200.28	503.13	182.46	281.77	315.87	168.35	428.87	0.27	1.88
		60	520.62	332.07	226.93	555.06	197.43	305.24	351.49	181.15	463.77	0.28	1.94
L1 ₂ -	GGA	0	133.30	78.06			42.06		96.47	35.53	94.95	0.34	2.71
Ga ₃ Zr		10	174.39	118.48			59.73		137.12	44.04	119.34	0.35	3.11
		20	224.87	152.03			82.24		176.31	59.31	159.99	0.35	2.97
		30	282.63	182.98			103.97		216.20	77.39	207.42	0.34	2.79
		40	330.22	214.98			122.31		253.39	90.42	242.42	0.34	2.80
		50	365.04	247.41			137.82		286.62	97.93	263.76	0.35	2.93
		60	409.99	280.78			152.77		323.85	108.16	291.99	0.35	2.99
	LDA	0	149.19	95.33			50.32		113.28	39.15	105.33	0.35	2.89
		10	197.38	135.00			71.18		155.79	51.12	138.23	0.35	3.05
		20	255.69	168.39			95.20		197.49	69.62	186.89	0.34	2.84
		30	313.31	200.50			115.70		238.10	86.72	231.99	0.34	2.75
		40	356.32	234.42			133.04		275.05	97.26	261.01	0.34	2.83
		50	394.90	268.83			148.30		310.85	105.21	283.64	0.35	2.95
		60	435.20	303.04			162.27		347.09	113.17	306.24	0.35	3.07

Table 3 Elastic constants C_{ij} , bulk modulus *B*, shear modulus *G*, Young's modulus *E* (all in GPa), Poisson's ratio *v* and Elastic anisotropy index A^U of $D0_{22}$ - and $L1_2$ -Ga₃Zr under various pressures

The hardness and brittleness of the compounds also have a relation to the ratio (*B/G*) between bulk modulus and shear modulus. According to Pugh's criterion [30], the compound with larger *B/G* ratio (> ~1.75) usually is ductile, and with smaller *B/G* ratio (< ~1.75) usually is brittle. Our calculated *B/G* values of Ga₃Zr are illustrated in Fig. 1. From Table 3 and Fig. 1, one can find that, the ratio B/G of $D0_{22}$ - and $L1_2$ -Ga₃Zr will become larger with pressure going up, it indicates that better ductility can be anticipated for the both structures of Ga₃Zr under high pressures. However, for $D0_{22}$ -Ga₃Zr, the ratio of B/G constantly increases with the pressure going up. Meanwhile, for $L1_2$ -Ga₃Zr, a sharply increasing of B/G is followed by a decreasing in pressure range of 10~30 GPa, and then a gradual increasing from 30 GPa to 60 GPa.

Besides that, the B/G values of $L1_2$ -Ga₃Zr are larger than 1.75, while the values of $D0_{22}$ -Ga₃Zr are much lower, it can be interpreted that $L1_2$ -Ga₃Zr will exhibit better ductility than $D0_{22}$ -Ga₃Zr in the pressure range of 0~60 GPa.

Furthermore, for $D0_{22}$ -Ga₃Zr, the *B/G* values is lower than 1.75 in the pressure range from 0 GPa to ~35 GPa, while larger than 1.75 in the range from ~35 GPa to 60 GPa. It suggests that $D0_{22}$ -Ga₃Zr will change from brittle to ductile when pressure is higher than ~35 GPa.



Figure 1. Raito between bulk modulus (*B*) and shear modulus (*G*) of $D0_{22}$ - and $L1_2$ -Ga₃Zr under various pressures (the horizontal dash line denote the value of B/G = 1.75).

Debye temperature. Debye temperature (Θ_D) is a fundamental parameter for the materials' thermodynamic properties, and it is correlated with many physical properties such as specific heat, elastic constants, melting temperature, etc. The experimental value of a solid usually can be calculated from the sound velocity [31]. In this paper, Debye temperatures of $L1_2$ - and $D0_{22}$ -Ga₃Zr under zero and high pressures are estimated with the elastic constant data. Θ_D can be ascertained from the averaged sound velocity by the following equation [31]:

$$\Theta_{\rm D} = \frac{h}{k} \left[\frac{3n}{4\pi} \left(\frac{N_{\rm A} \rho_0}{M} \right) \right]^{\frac{1}{3}} v_{\rm m} \tag{2}$$

where *h* is the Planck's constant, *k* is Boltzmann's constant, N_A is the Avogadro constant, *n* is the atoms number per molecule, *M* is the molecular weight, and ρ_0 is the density, respectively. The average sound velocity v_m can be calculated as follows:

$$v_{\rm m} = \left[\frac{1}{3} \left(\frac{2}{v_{\rm s}^3} + \frac{1}{v_{\rm l}^3}\right)\right]^{-1/3}, \text{ and } v_{\rm l} = \left(\frac{3B + 4G}{3\rho_0}\right)^{1/2}, v_{\rm s} = \left(\frac{G}{\rho_0}\right)^{1/2}$$
(3)

where v_1 and v_s are longitudinal and shear sound velocities, respectively. The Debye temperatures of $L1_2$ - and $D0_{22}$ -Ga₃Zr are calculated from the aforementioned values of lattice parameters, bulk modulus and shear modulus, and the results are listed in Table 4.

Table 4 Debye temperature Θ_D (unit in K) of $D0_{22}$ - and $L1_2$ -Ga₃Zr under various pressures

Dhagag	VC	Pressure (GPa)								
Fliases	AC	0	10	20	30	40	50	60		
$D0_{22}$ -Ga ₃ Zr	GGA-PBE	409.62	460.40	493.92	527.07	550.43	573.41	593.13		
	LDA-CAPZ	440.24	475.97	516.57	543.63	567.77	589.12	608.51		
$L1_2$ -Ga ₃ Zr	GGA-PBE	287.48	316.21	362.75	410.38	440.45	455.93	476.72		
	LDA-CAPZ	298.34	337.02	389.11	430.64	453.38	469.19	484.55		



Figure 2. Dependence of Debye temperature (Θ_D) as function of pressure for $D0_{22}$ - and $L1_2$ -Ga₃Zr.

In Debye theory, Θ_D is the temperature of a crystal's highest normal mode of vibration, i.e., the highest temperature that can be achieved due to a single normal vibration. One can find that the Debye temperatures of both structures will increase with the pressure increasing, which indicates that the normal vibration of both crystals will enhance when the pressure increases. The $D0_{22}$ -Ga₃Zr has higher Θ_D than $L1_2$ -Ga₃Zr, and the gap of Θ_D between the both phases constantly maintains as pressure increasing.

Summary

The elastic constants, mechanical moduli, Debye temperature of $D0_{22}$ - and $L1_2$ -Ga₃Zr have been investigated with external pressure varying from 0 GPa to 60 GPa by performing DFT calculations. The results show that (1) elastic constants and mechanical moduli increase with pressure's going up; (2) the ductility of $L1_2$ -Ga₃Zr is larger than $D0_{22}$ -Ga₃Zr, and the ductility of the both phases will roughly increase with pressure's increasing, and the transition of $D0_{22}$ -Ga₃Zr from brittle to ductile will take place at about 35 GPa; (3) the Debye temperature of the both phases will increase along with pressure going up, and $D0_{22}$ -Ga₃Zr has higher Debye temperature than $L1_2$ -Ga₃Zr.

Acknowledgements

The authors acknowledge the technical support from Center for High Performance Computing of Northwestern Polytechnical University, and the financial support from Scientific Research Program Funded by Shaanxi Provincial Education Department (15JK1570), Technology Creative Foundation of Xi'an Shiyou University (2015BS12), PetroChina Innovation Foundation (2013D-5006-0601), and National college students' innovative entrepreneurial training program funded projects (201410705030).

References

[1] Z. Zhang, L. Stixrude and J. Brodholt: Earth and Planetary Science Letters, Vol. 379 (2013), p.1.

[2] Z. Jiao, S. Ma, X. Zhang and X. Huang: EPL (Europhysics Letters), Vol. 101 (2013) No.4, p.46002.

[3] A. H. Reshak, I. V. Kityk, J. Ebothe, A. O. Fedorchuk, M. F. Fedyna, H. Kamarudin and S. Auluck: Journal of Alloys and Compounds, Vol. 546 (2013) p.14.

[4] A. H. Reshak, G. Lakshminarayana, J. Ebothe, A. O. Fedorchuk, M. F. Fedyna, H. Kamarudin, P. Mandracci and S. Auluck: Journal of Alloys and Compounds, Vol. 556 (2013) p.259.

[5] W. Luo, S. Liu, Y. Tang, M. Yin, B. Sundman, Y. Du, P. Nash and H. Tao: Journal of Alloys and Compounds, Vol. 587 (2014) p.497.

[6] H. J. Wallbaum: Zeitschrift Fur Metallkunde, Vol. 34 (1942) p.118.

[7] S. J. Clark, M. D. Segall, C. J. Pickard, P. J. Hasnip, M. J. Probert, K. Refson and M. C. Payne: Zeitschrift fuer Kristallographie, Vol. 220 (2005) No.5-6, p.567.

[8] M. D. Segall, P. J. D. Lindan, M. J. Probert, C. J. Pickard, P. J. Hasnip, S. J. Clark and M. C. Payne: Journal of Physics: Condensed Matter, Vol. 14 (2002) No.11, p.2717.

[9] K. Laasonen, A. Pasquarello, R. Car, C. Lee and D. Vanderbilt: Physical Review B, Vol. 47 (1993) p.10142.

[10]D. Vanderbilt: Physical Review B, Vol. 41 (1990) No.11, p.7892.

[11] J. P. Perdew, K. Burke and M. Ernzerhof: Physical Review Letters, Vol. 77 (1996) No.18, p.3865.

[12] J. P. Perdew and A. Zunger: Physical Review B, Vol. 23 (1981) No.10, p.5048.

[13] D. M. Ceperley and B. J. Alder: Physical Review Letters, Vol. 45 (1980) No.7, p.566.

[14] H. G. von Schnering and R. Nesper: Acta Chemica Scandinavica, Vol. 45 (1991) No.8, p.870.

[15] J. Goldak, L. T. Lloyd and C. S. Barrett: Physical Review, Vol. 144 (1966) p.478.

[16]S. Kurth, J. P. Perdew and P. Blaha: International Journal of Quantum Chemistry, Vol. 75 (1999) No.4-5, p.889.

[17] F. Gao, E. J. Bylaska and W. J. Weber: Physical Review B, Vol. 70 (2004) p.245208.

[18] D. J. Siegel, L. G. Hector and J. B. Adams: Surface Science, Vol. 498 (2002) No.3, p.321.

[19] R. Ahmed, Fazal-e-Aleem, S. J. Hashemifar and H. Akbarzadeh: Physica B-Condensed Matter,

Vol. 403 (2008) No.10-11, p.1876.

[20]A. J. Du, S. C. Smith, X. D. Yao and G. Q. Lu: Journal of Physical Chemistry B, Vol. 109 (2005) No.38, p.18037.

[21]G. Ghosh, S. Vaynman, M. Asta and M. E. Fine: Intermetallics, Vol. 15 (2007) No.1, p.44.

[22] P. Tang and B. Tang: Solid State Communications, Vol. 152 (2012) No.21, p.1939.

[23] A. Jahn, M. Tek, I. Krajccaron, M. and J. Hafner: Physical Review B, Vol. 71 (2005) No.2, p.24101.

[24] Y. Duan, Y. Sun, M. Peng and Z. Guo: Solid State Sciences, Vol. 13 (2011) No.2, p.455.

[25] J. Haines, J. M. Léger and G. Bocquillon: Annual Review of Materials Research, Vol. 31 (2001) No.1, p.1.

[26] J. P. Watt and L. Peselnick: Journal of Applied Physics, Vol. 51 (1980) No.3, p.1525.

[27] A. I. Lurie: Theory of Elasticity (Springer, Germany 2005).

[28]C. Li and P. Wu: Chemistry of Materials, Vol. 13 (2001) No.12, p.4642.

[29]L. Fu, J. Ke, Q. Zhang, B. Tang, L. Peng and W. Ding: Physica Status Solidi B-Basic Research, Vol. 249 (2012) No.8, p.1510.

[30] S. F. Pugh: Philosophical Magazine, Vol. 45 (1954) No.367, p.823.

[31]G. Grimvall: Thermophysical Properties of Materials (Elsevier, Netherlands 1999).