Theoretical investigations of physical properties of $MNNi_3$ (M=Zn, Mg, Al) under pressure

XIAOFENG LI[a*], LIU XIUYING[b], HONGCUN ZHAI[c], GUANGFU JI[d]
[a]*College of Physics and Electronic Information, Luoyang Normal College, Luoyang 471022, PR China*
[b]*College of Science, Henan University of Technology, Zhengzhou 450000, PR China*
[c]*Mathematics College, Luoyang Normal College, Luoyang 471022, PR China*
[d]*Laboratory for Shock Wave and Detonation Physics Research, Institute of Fluid Physics, Chinese Academy of Engineering Physics, Mianyang 621900, PR China*

The elastic and thermodynamic properties of the antiperovskite superconductor $MNNi_3$ (M=Zn, Mg, Al) are investigated by first-principles calculations. The calculated structural parameters and elastic properties of $MNNi_3$ are in good agreement with experimental data and the available theoretical data. From the high pressure elastic constants, $ZnNNi_3$, $MgNNi_3$ and $AlNNi_3$ are predicted that they are not stable at a pressure above 61.2GPa, 113.3GPa and 122.4GPa, respectively. By the Debye model, the thermodynamic properties such as the Grüneisen parameter γ and bulk modulus (B_T and B_S) under pressures and temperatures are also successfully obtained.

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1. Introduction

Soon after the discovery of 8 K in Ni-rich intermetallic antiperovskite superconductor compound $MgCNi_3$ [1], a lot of attentions have been aroused on the iso-structural cubic antiperovskites for their many puzzling physical properties and important technical applications. The compound has the classical cubic perovskite structure with space group *Pm-3m*. At the same time, many researchers have been focused on the development of design principles, synthesis and investigations of related antiperovskite-type carbides. So many cubic antiperovskites have been synthesized and their physical properties have been investigated, such as (Mg, Zn) CNi_3 [2], (Al, Ga, Cd)CNi_3 [3-5] and $In_{0.95}CNi_3$ [6]. It is noteworthy that only $MgCNi_3$ and $CdCNi_3$ indicate superconductivity. Theoretical calculations of these antiperovaskite [7-12] showed a large narrow density of states (DOS) peak in the vicinity of the Fermi level (E_F). The DOS at E_F is not large enough to induce magnetic instability [13], but is associated with the superconducting properties [11]. Numerous efforts [13–18] have been made with hole-doped $MgCNi_3$ in an attempt to shift the Fermi level, thereby leading an increase of the DOS at E_F, whereupon *T*c was found to decrease. However, some groups successfully enhanced the T_c by using pressure, but the cause is still controversial and remains an open problem [16, 17]. Kumary *et al* [13] considered that a lattice softening or a structural phase transition lead enhancement of T_C under pressure. Zhang et al [18] investigated the elastic constants and electronic structures of $MgCNi_3$ under pressure, they found $MgCNi_3$ is not stable above 58.4GPa and analyzed the cause of the enhancement of T_c with pressure.

Very recently, a first new superconducting (T_C~3K) Ni-rich nitrogen-containing antiperovskite $ZnNNi_3$ has been successfully synthesized by replacing carbon by nitrogen [19]. It provides another route of synthesizing superconducting compound though its superconducting temperature is very low. Due to a great deal of attentions on antiperovskite $ZnNNi_3$, several research groups have investigated the physical properties of $ZnNNi_3$ [20-23]. However , these authors only studied the structural properties and electronic structure of $MNNi_3$ at zero pressure, there are few investigations on the properties of $MNNi_3$(M=Zn, Al, Mg) under pressures. Especially the elastic constants under pressure are very important to determine anisotropies and thermodynamic properties; the electronic structure under pressures is associated with the superconducting temperature. Therefore, it is very significant to investigate mechanical stability, elastic and thermodynamic properties of $MNNi_3$ under pressure.

2. Theoretical methods

2.1. Total energy electronic structure calculations

In the electronic structure calculations, the ultrasoft pseudopotentials introduced by Vanderbilt [24] have been employed for all the ion-electron interaction. The effects of exchange-correlation interaction are treated within the generalized gradient approximation of Perdew, Burke, and Ernzerhof (GGA-PBE) [25]. A plane wave basis set with

cut-off energy 800.00 eV is applied. Pseudo atomic calculations are performed for Zn $3d^{10}4s^2$, Mg $2p^6$ $3s^2$, Al $3s^2$ $3p^1$, Ni $3d^8$ $4s^2$ and N $2s^22p^3$. As for the Brillouin-zone sampling, we use the 12×12×12 k-points. The self-consistent convergence of the total energy is at 10^{-7} eV/Atom. Hydrostatic pressure, coupled with the variable cell approach, is applied within the Parrinello–Rahman method to perform a full optimization of the cell structure for each target external pressure. All these total energy electronic structure calculations are implemented by using the CASTEP code [26, 27].

2.2 Elastic properties

To calculate the elastic constants under pressure, we applied the volume-conserving method. The complete elastic constant tensor was determined from calculations of the stresses induced by small deformations of the equilibrium primitive cell, The elastic constants C_{ijkl} are then determined as [28-30]:

$$c_{ijkl} = (\frac{\partial \sigma_{ij}(x)}{\partial e_{kl}})_X \tag{1}$$

where s_{ij} and e_{kl} are the applied stress and Eulerian strain tensors, and X and x are the coordinates before and after the deformation. For the isotropic stress, the elastic constants are defined as [29-31]:

$$c_{ijkl} = C_{ijkl} + \frac{P}{2}(2\delta_{ij}\delta_{kl} - \delta_{il}\delta_{jk} - \delta_{ik}\delta_{jl}) \tag{2}$$

$$C_{ijkl} = (\frac{1}{V(x)}\frac{\partial^2 E(x)}{\partial e_{ij}\partial e_{kl}})_X \tag{3}$$

where C_{ijkl} is the second-order derivatives with respect to the infinitesimal strain (Eulerian). For cubic crystals $MNNi_3$, there are three independent elastic constants, *i.e.* C_{11}, C_{12}, C_{44}.

For a cubic structure $MNNi_3$, the bulk modulus B, the shear modulus G and the Young's modulus E are taken as

$$B = (C_{11} + 2C_{12})/3 \tag{4}$$

$$G = \left(3C_{44} + C_{11} - C_{12}\right)/5 \tag{5}$$

$$E = \frac{9BG}{3B+G} \tag{6}$$

The Debye temperature may be estimated from the average sound velocity V_m [32]:

$$\Theta = \frac{h}{k}\left[\frac{3n}{4\pi}\left(\frac{N_A\rho}{M}\right)\right]^{1/3} V_m \tag{7}$$

where h is Planck's constants, k is Boltzmann's constant, N_A is Avogadro's number, n is the number of atoms per formula unit, M is the molecular mass per formula unit, ρ is the density, and V_m is obtained from [32]

$$V_m = \left[\frac{1}{3}\left(\frac{2}{V_s^3} + \frac{1}{V_l^3}\right)\right]^{-1/3} \tag{8}$$

where V_s and V_l are the shear and longitudinal sound velocities, respectively, which can be related to the shear and bulk moduli by the Navier's equations [33]:

$$V_s = \sqrt{\frac{G}{\rho}} \quad , \quad V_l = \sqrt{(B + \frac{4}{3}G)/\rho} \tag{9}$$

2.3 Thermodynamic properties

To investigate the thermodynamic properties of $MNNi_3$, we apply the quasi-harmonic Debye model [34], in which the phononic effect is considered, and the non-equilibrium Gibbs function $G^*(V; P, T)$ takes the form of

$$G^*(V;P,T) = E(V) + PV + A_{Vib}(\Theta(V);T) \tag{10}$$

where $E(V)$ is the total energy per unit cell, PV corresponds to the constant hydrostatic pressure condition, $\Theta(V)$ is the Debye temperature, and A_{vib} is the vibrational Helmholtz free energy that can be written as

$$A_{Vib}(\Theta;T) = nkT[\frac{9}{8}\frac{\Theta}{T} + 3\ln(1-e^{-\Theta/T}) - D(\Theta/T)] \tag{11}$$

with the $D(\Theta/T)$ representing the Debye integral, n denoting the number of atoms per formula unit, and Θ is the Debye temperature.

By solving the following equation with respect to V

$$\left(\frac{\partial G^*(V;P,T)}{\partial V}\right)_{P,T} = 0 \tag{12}$$

one could obtain the thermal equation of state, V (P, T) and the thermal expansion coefficient α as follows

$$\alpha = \gamma C_V / (B_T V) \tag{13}$$

where the isothermal bulk modulus B_T, the heat capacity C_V and the Grüneisen parameter γ are expressed as

$$B_T(P,T) = V[\frac{\partial^2 G^*(V;P,T)}{\partial^2 V^2}]_{P,T} \tag{14}$$

$$\gamma = -\frac{d\ln\Theta(V)}{d\ln V} \tag{15}$$

3. Results and discussions

3.1 Structural properties

For the non-oxide perovskite-type superconductor $MNNi_3$, a series of lattice constant a are set to calculate the total energy E and the corresponding primitive cell volume V, and then the obtained E-V data is fitted to the Birch-Murnaghen equation of state (EOS) [35]. The obtained equilibrium lattice constants a, zero-pressure bulk modulus B_0 and its pressure derivation B_0' of $MNNi_3$ (M=Zn, Al, Mg) at P=0 and T=0 are summarized in Table 1, together with other theoretical [20-23] and experimental data [19]. In Table 1, it is easily found that the calculated values are in good consistent with the obtained theoretical [20-23] and experimental data [19]. Simultaneously, the bond lengths of Zn-Ni, N-Ni are also showed in Table 1. It is found that the relations of the bond length in $MNNi_3$ are:

$$d_{\text{Zn-Ni}} < d_{\text{Al-Ni}} < d_{\text{Mg-Ni}}, \quad d_{\text{N-Ni}}(ZnNNi_3) < d_{\text{N-Ni}}(AlNNi_3) < d_{\text{N-Ni}}(MgNNi_3)$$

Unfortunately, to our best knowledge, no experiment data for bulk modulus and bond length of $MNNi_3$ are available to be compared with our theoretical results.

Table 1 The calculated equilibrium parameter a (Å), bulk modulus B_0 (GPa), pressure derivative bulk modulus B_0' and the bond length $ZnNNi_3$, $MgNNi_3$, and $AlNNi_3$ at P=0 and T=0, respectively.

$MNNi_3$		Present work	Other work
$ZnNNi_3$	a	3.765(3.756[a])	3.77[b], 3.770[c] 3.719[d], 3.769[e]
	B_0	192.1	198.92[b] 225.61[d]
	B_0'	4.97	4.75[d]
	$d_{\text{Zn-Ni}}$	2.681	
	$d_{\text{N-Ni}}$	1.896	
$MgNNi_3$	a	3.841	3.82[b], 3.815[c]
	B_0	169.3	188.53[b]
	B_0'	4.80	
	$d_{Mg\text{-}Ni}$	2.715	
	$dN\text{-}Ni$	1.920	
$AlNNi_3$	a	3.794	3.777[c]
	B_0	197.6	
	B_0'	4.82	
	$d_{Al\text{-}Ni}$	2.683	
	$d_{N\text{-}Ni}$	1.897	

[a] Ref [19](experiment data) [b] Ref[20] [c]Ref [21] [d] Ref [22] [e] Ref [23]

3.2 Elastic constants and mechanical stability under pressure

The elastic constants of solids provide a link between the mechanical and dynamical behaviors of crystals, and give important information concerning the nature of the forces operating in solids. The elastic constants of C_{11}, C_{12} and C_{44} are listed in Table 2. It is shown that the differences between our results and Li *et al* [20] are a bit large. Since there are no experimental data to compare with, we listed the available theoretical data of $ZnNNi_3$. The lattice parameters from our calculations seem to be better than those by Li *et al*. Then we think that our calculations for elastic constants should be more reliable.

Table 2 The calculated elastic constants C_{11}, C_{12}, C_{44}, bulk modulus B, shear and Young modulus(GPa), B/G and Debye temperature Θ_D(K).

		C_{11}	C_{12}	C_{44}	B	G	E	B/G	Θ_D
$ZnNNi_3$	present	321.7	125.1	35.4	190.6	54.1	251.6	3.52	315
	other cal.	354.28[a]	134.01[a]	48.06[a]	207.43[a]	48.06[a]	229.1[a]		276.47e
		381.6[b]	116.5[b]	17.9[b]					271.57[f]
		364.2[c]	124.9[c]	32.69[c]					287.49[g]
		394.57[d]	140.28[d]	55.39[d]					336[h]
$MgNNi_3$	present	317.8	112.4	55.8	180.8	69.6	259.1	2.59	397
	other cal.	336.19[a]	125.31[a]	48.96[a]	195.60[a]	48.96[a]			
$AlNNi_3$	present	354.7	122.4	50.0	199.9	70.6	290.9	2.83	391
	other cal.	431.4[b]	96.1[b]	48.0[b]	207.8[b]	81.5[b]	216.3[b]		

[a] Ref [19](experiment data) [b] Ref[20] [c] Ref [21] [d] Ref [22] [e] GGA-WC, Ref[22] [f] GGA-PBE, Ref[22] [g] LDA, Ref[22] [h] Ref[19]

The elastic constants are estimated from first principles calculations for cubic $MNNi_3$ perovskite. However, the materials are often used in polycrystalline aggregates; therefore it is useful to estimate the corresponding parameters of the polycrystalline species. For these purposes we have utilized the Voigt-Reuss-Hill approximation to calculate the main mechanical parameters for cubic $MNNi_3$ perovskite (Table 2), namely, bulk modulus B, shear modulus G and Young's modulus E from the elastic constants of the single crystals. The bulk modulus B of $MNNi_3$ (M=Zn, Mg, Al) are in good agreement with the ones obtained from the equation of state fitting. It may be an estimation of the reliability and accuracy of our calculated elastic constants for $MNNi_3$.

The ratio between the bulk and the shear modulus, B/G, has been proposed by Pugh to predict brittle or ductile behavior of materials. The shear modulus G represents their resistance to plastic deformation, while B represents their resistance to fracture. A high B/G ratio is associated with ductility, whereas the low value corresponds to the brittle nature. The critical value which separate ductile and brittle materials is around 1.75, i.e., if B/G>1.75, the material behaves in ductile manner, otherwise the materials behaves in brittle manner. We have found that B/G rations are 3.52, 2.59, 2.83 for $MNNi_3$ (M=Zn, Mg, Al) (also listed in Table 2) respectively, indicating that $MNNi_3$ are ductile.

The Debye temperature is one of the important thermodynamic parameters and is closely related to many thermophysical properties of solids, such as specific heat, thermal expansion, vibrational entropy, sound velocities, hardness and melting temperature. The Debye temperatures Θ_D of $MNNi_3$ are obtained from Eq. (7)-Eq. (9) , which are also listed in Table 2, together with other experimental[19] and theoretical data [22]. The calculated Debye temperature Θ_D of $ZnNNi_3$ is 315K, which is more closely to the experimental data than other theoretical data. The Debye temperatures in $ZnNNi_3$, $AlNNi_3$ and $MgNNi_3$ gradually increase.

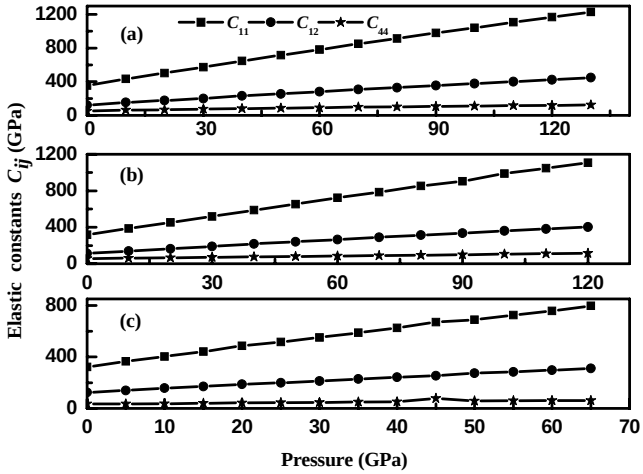

Fig. 1 The dependence of C_{ij} of $MNNi_3$ on pressure.

The elastic constants of $MNNi_3$ under pressure, obtained for the first time, are illustrated in Fig. 1. It is seen that C_{11}, C_{12} and C_{44} increase with the enhancement of pressure. The change of C_{11} is more sensitive to pressure than other three, while C_{44} is the most unresponsive one. Recently, elastic constants and mechanical stabilities of crystals have attracted lots of interest from physicists. In 2002, Sin'ko and Smirov [36] deduced the conditions of mechanical stability from elastic constants. As is known, for a cubic crystal, the mechanical stability under isotropic pressure is judged from the following condition:

$$\widetilde{C}_{44}>0,\ \widetilde{C}_{11}>|\widetilde{C}_{12}|,\ \widetilde{C}_{11}+2\widetilde{C}_{12}>0, \qquad (16)$$

where $C_{\alpha\alpha} = C_{\alpha\alpha} - P$ (α =1, 4), $C_{12} = C_{12} + P$. By

fitting $\widetilde{C}_{44}$ data to second-order polynomials, we have the following relations

$$\widetilde{C}_{44} = \alpha + \beta P - \gamma P^2. \quad (17)$$

Fig. 2 shows the $\widetilde{C}_{44}$ versus pressure for $MNNi_3$ (M=Zn, Mg, Al). When $\widetilde{C}_{44} > 0$ is no longer fulfilled, indicating that $MNNi_3$ is not mechanical stable at pressures above the pressure of $\widetilde{C}_{44} = 0$. The critical pressures of $MNNi_3$ (M=Zn, Mg, Al) are 61.2GPa, 113.3GPa and 122.4GPa, respectively. In our former work, the obtained critical pressure of $MgCNi_3$ is 58.4GPa [18], which is reasonable by comparing some experimental data. In fact, according to our experience, the phase transition pressure should be smaller than the critical mechanical stable pressure.

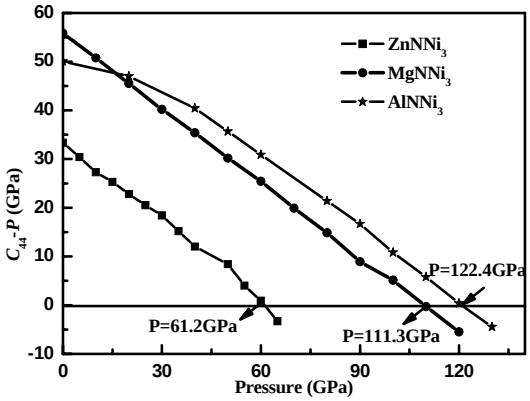

Fig. 2 The mechanical stability of $MNNi_3$ versus pressure at 0 K.

3.3 Thermodynamic properties

Through the quasiharmonic Debye model, one can calculate the thermodynamic quantities of cubic $MNNi_3$ at any temperature and pressure from the *E-V* data calculated at T =0 and P =0. The dependences of isothermal and adiabatic bulk moduli (B_T, B_S) of $MNNi_3$ on temperature are illustrated in Fig. 3. It is easily seen that the isothermal and adiabatic bulk moduli (B_T, B_S) gradually increases with temperature in $MgNNi_3$, $ZnNNi_3$ and $AlNNi_3$. It also can be found that B_T and B_S are nearly constant from 0 K to 100K and then decrease almost linearly with increasing temperatures, as is obvious from the relationship $B_S = B_T(1 + \alpha\gamma T)$. B_T and B_S coincide at low temperature and then diverge with rising T. It is found that the relationships between bulk modulus and pressure are nearly linear at various temperatures. However, the variety of dB_T/dT is much stronger than that of dB_S/dT.

The Grüneisen parameter γ could describe the alteration in vibration of a crystal lattice based on the increase or decrease in volume as a result of temperature change. Recently, it has been widely used to characterize and extrapolate the thermodynamic properties of materials at high pressures and high temperatures. In Fig.4, the variation of Grüneisen parameter γ with pressure and temperature are displayed, from which it can be found that the Grüneisen parameter γ decrease exponentially as the pressure increases, however, as the temperature enhanced Grüneisen parameter γ increase fast. It is also seen that Grüneisen parameter γ of $ZnNNi_3$ is bigger than that of $MgNNi_3$ and $AlNNi_3$. Moreover, the Grüneisen parameter of $MgNNi_3$ is nearly the same as $AlNNNi_3$ with temperature up to 1000K.

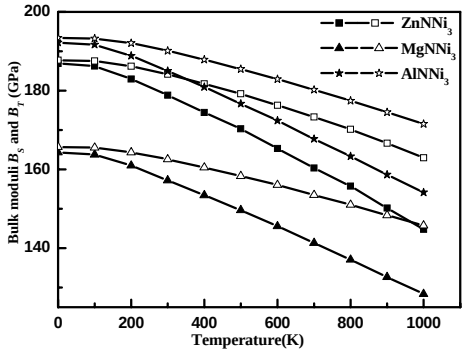

Fig.3 Temperature dependence of isothermal (B_T =solid) and adiabatic (B_S=hollow) zero-pressure bulk modulus of $MNNi_3$.

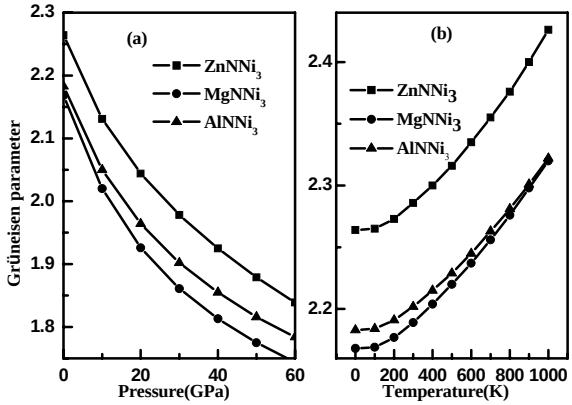

Fig. 4. The Grüneisen parameter γ of $MNNi_3$ versus pressure(a) at 0K and temperature (b) at 0GPa.

4. Conclusions

The structural, elastic properties, mechanical stability and thermodynamic properties of the anti-perovskite superconductor $MNNi_3$ (M=Zn, Mg, Al) under pressure are investigated by first-principles calculations with the generalized gradient approximation for exchange and correlation for the first time. The calculated structural parameters elastic properties of $MNNi_3$ are in good agreement with experimental data and the available theoretical data. From the high pressure elastic constants,

$ZnNNi_3$, $MgNNi_3$ and $AlNNi_3$ are predicted that they are not stable at a pressure above 61.2GPa, 113.3GPa and 122.4GPa, respectively. Finally, the thermodynamic properties such as the Grüneisen parameter and bulk modulus (B_T and B_S) under pressures and temperatures are also successfully obtained. By the present work, the mechanical behaviors of $ZnNNi_3$, $MgNNi_3$ and $AlNNi_3$ show very big similarity. It should be used to stimulate future experimental and theoretical work.

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Reference

[1] T. He, Q. Huang, A. P. Ramirez, Y. Wang, K. A. Regan, N. Rogado, M. A. Hayward, M. K. Haas, J. S. Slusky, K. Inumara, H.W. Zandbergen, N. P. Ong and R. J. Cava, Nature **411,** 54 **(**2001).
[2] M. Uehara, T. Yamazaki, T. Krôi, T. Kashida, Y. Kimishima, K. Ohishi, J. Phys. Chem. Solids **68,** 2178(2007).
[3] A. F. Dong, G. C. Che, W. W. Huang, S. L. Jia, H. Chen, Z. X. Zhao, Physica C **422**, 65 (2005).
[4] P. Tong, Y. P. Sun, X. B. Zhu, W. H. Song, Phys. Rev. B **73,** 245106 (2006).
[5] M. Uehara, T. Yamazaki, T. Kori, T. Kashida, Y. Kimishima, I. Hase, J. Phys. Soc. Japan **76,** 034714 (2007).
[6] P. Tong, Y. P. Sun, X. B. Zhu, W. H. Song, Solid State Commun. **141,** 336 (2007).
[7] J. H. Shim, S. K. Kwon, B. I. Min, Phys. Rev. B **64,** 180510(R) **(**2001).
[8] D. J. Singh, I. I. Mazin, Phys. Rev. B **64,** 140507(R) (2001).
[9] S. B. Dugdale, T. Jarlborg, Phys. Rev. B **64,** 100508 (R) (2001).
[10] A. Szajek, J. Phys.: Condens. Matter **13,** L595 (2001).
[11] I. R. Shein, A. L. Ivanovskii, N. I. Medvedeva, JETP Lett. **74,** 122 (2001).
[12] H. Rosner, R. Weht, M. D. Johannes, W. E. Pickett, E. Tosatti, Phys. Rev. Lett. **88,** 027001 **(**2002**)**.
[13] T. G. Kumary, J. Janaki, A. Mani, S. M. Jaya, V. S. Sastry, Y. Hariharan, T. S. Radhakrishnan, M. C. Valsakumar, Phys. Rev. B **66,** 064510 (2002).
[14] A. Das, R. K. Kremer, Phys. Rev. B **68**, 064503 (2003).
[15] T. Klimczuk, V. Gupta, G. Lawes, A. P. Ramirez, R. J. Cava, Phys. Rev. B **70,** 094511 (2004).
[16] C. Sulkowski, T. Klimczuk, R. J. Cava, K. Rogacki, Phys. Rev. B **76,** 060501(R) **(**2007).
[17] H. D. Yang, S. Mollah, W. L. Huang, P. L. Ho, H. L. Huang, C. J. Liu, J. Y. Lin, Y. L. Zhang, R. C. Yu, C. Q. Jin, Phys. Rev. B **68,** 092507 (2003).
[18] W. Zhang, X. R. Chen, L. C. Cai, F. Q. Jing, J. Phys.: Condens. Matter **20,** 325228 (2008).
[19] M. Uehara, A. Uehara, K. Kozawa, Y. Kimishima, J. Phys. Soc. Japan **78**, 033702 (2009).
[20] C. Li, W. G. Chen, F. Wang, S. F. Li, Q. Sun, S.Y. Wang, Y. Jia, J. Appl. Phys. **105,** 123921 (2009).
[21] V. V. Bannikov, I. R. Shein, A. L. Ivanovskii, Physica B **405**, 4615 (2010).
[22] C. M. I. Okoye, Physica B **405,** 1562 (2010).
[23] I. R. Shein, V. V. Bannikov, A. L. Ivanorski, e-print arXiv: cond-mat/0811.4249.
[24] D. Vanderbilt, Phys. Rev. B **41**, 7892 (1990).
[25] J. P. Perdew, Y. Wang, Phys. Rev. B **45,** 13244 (1992).
[26] M. C. Payne, M. P. Teter, D. C. Allen, T. A. Arias, J. D. Joannopoulos, Rev. Mod. Phys. **64,** 1045 (1992).
[27] V. Milman, B. Winkler, J. A. White, C. J. Packard, M. C. Payne, E. V. Akhmatskaya, R. H. Nobes, Int. J. Quantum Chem. **77,** 895 (2000).
[28] J. Wang, S. Yip, S. R. Phillpot, D. Wolf, Phys. Rev. B **52,** 12627 (1995).
[29] D. C. Wallace, Thermodynamics of Crystals (Wiley, New York, 1972).
[30] B. B. Karki, G. J. Ackland, J. Crain, J. Phys.: Condens. Matter **9,** 8579 (1997).
[31] T. H. K. Barron, M. L. Klein, Proc. Phys. Soc. **85,** 523 (1965).
[32] O. L. Anderson, J. Phys. Chem. Solids **24,** 909 (1963).
[33] E. Schreiber, O.L. Anderson, N. Soga, Elastic Constants and their Measurements (New York: McGraw-Hill, 1973).
[34] E. Francisco, J.M. Recio, M.A. Blanco, A. Martín—Pendás and A. Costales, J. Phys. Chem. **102,** 1595 (1998).
[35] F. D. Murnaghan, Proc. Natl. Acad. Sci. USA. **30,** 244 (1944).
[36] G. V. Sin'ko, N. A. Smirnov, J. Phys.: Condens. Matter **14,** 6989 (2002).

*Corresponding author: lxfdjy@126.com