

Elastic and thermodynamic properties of VN under pressure and effect of metallic bonding on its hardness^{*}

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By the *particle-swarm optimization* method, it is predicted that tetragonal P4₂mc, I4₁md and orthorhombic Amm2 phases of Vanadium nitride (VN) are energetically stable than NaCl type structure at 0 K. The enthalpy of the predicted three new VN phases, along with WC, NaCl, AsNi, CsCl type structures, have been calculated as a function of pressure. We found that VN performs the WC to CsCl type phase transition at 256 GPa. For the considered seven crystallographic VN phases, the structures, elastic constants, bulk modulus, shear modulus and Debye temperatures have been investigated, our calculated equilibrium structural parameters are in very good agreement with the available experimental results and the previous theoretical results for NaCl phase. The Debye temperatures of VN in novel predicted three phases are all higher than the rest structures. Elastic constants, thermodynamic properties and elastic anisotropies of VN under pressures are obtained and the mechanical stability are analyzed in details based on the mechanical stability criteria. Moreover, the effect of metallic bonding on the hardness of VN has also been investigated, which shows that VN in P4₂mc, I4₁md and Amm2 phases are potential superhard phases. The further investigation in the experimental level is highly

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recommended to confirm our calculations presented in this paper.

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1. Introduction

Transition-metal nitrides have received more attention for being the powerful candidates of superhard materials and potential technological applications.^[1-5] There are lots of theoretical and experimental efforts focus on the transition-metal nitrides. Vanadium nitride (VN) adopting the NaCl type structure has been the leading subject of many investigations on such transition-metal compounds because of its high melting temperature, electrical conductivity, and chemical stability.^[6-7] However, phonon anomalies have been observed in substoichiometric NaCl type VN_x (x<1.0) at the X point of the Brillouin zone (BZ) by inelastic neutron diffraction measurements.^[8] And the phonon spectrum calculations of VN at 0 K revealed that this compound is dynamically instable.^[9] The stoichiometric VN was found to have enhanced stability in the WC type structure as compared to the NaCl type structure based on the total energy calculation with the first-principles method.^[10] It is also found that the total energy of AsNi and tetragonal (*P4*₂/*mcm*) phases is lower than that of NaCl phase at 0 K and 0 GPa. The stabilization of the NaCl type over WC type transition-metal compounds with nitrogen vacancies was only detected in experiments. Meanwhile, tetragonal and triclinic phases have also been detected in experiments.^[11] In addition, VN was predicted to undergo a structural transition from NaCl to CsCl type arrangement under high pressure.^[12] Despite of the amount of experimental and theoretical information accumulated on VN, to our knowledge, the structural and thermodynamic properties of VN in various structures have not been well understood yet, especially under high pressure. In order to fully exploit this material, it is necessary to search for the new phases of stoichiometric VN in the framework of a first-principles approach, in order to obtain a good understanding of the physical properties of VN in various phases, in particular of its structural and thermodynamic properties under high pressure.

In the present paper, tetragonal $P4_2mc$, $I4_1md$ and orthorhombic $Amm2$ phases of VN are predicted to be energetically more stable than NaCl type structure with pressure increasing. We describe the structure properties and the phase transition of VN in the novel predicted three phases, along with WC, NaCl, AsNi, and CsCl type structures, by the first-principles calculations. The elastic and thermodynamic behaviors under high pressure have also been reported. The purpose is to give comprehensive information on the structures and mechanical properties of VN. Moreover, it is to provide a further understanding of thermodynamic properties of VN in various structures under high pressure. On the other hand, we aim to provide powerful guidelines for future experimental investigations and we hope that such investigations can contribute some further understanding of the hardness of VN in considered structures.

2. Computational methods

In our calculations, candidate structure searches of stoichiometric VN were performed at 0 K using the particle-swarm optimization (PSO) method.^[13] The first-principles calculations are performed based on the density functional theory packaged in Cambridge Serial Total Energy Package (CASTEP).^[14] The conventional unit cells are used for seven structures of VN during the geometry optimization process. For the electronic and elastic-constants calculations, Norm-conserving pseudopotential^[15] are used and the exchange-correlation terms are considered by the Perdew-Berke-Ernzerhof (PBE) form of the generalized gradient approximation (GGA). While for the hardness calculations, the Ultrasoft Vanderbilt pseudopotential^[16] are used, instead. During the structure optimizations, the total energy is minimized by optimizing both the cell parameters and the atomic positions. All forces on atoms are less than 0.01 eV and a self-consistent field tolerance of 2.0×10^{-6} eV was used. To ensure the precision in our calculations, the plane-wave cutoff energy is 850 and 500 eV for Norm-conserving potential and Ultrasoft Vanderbilt potential, respectively. The following k points set have been generated using Monkhorst-Pack scheme:^[17] $17 \times 17 \times 14$ and $16 \times 16 \times 8$ for hexagonal WC and AsNi phases, respectively,

16×16×16 for cubic NaCl and CsCl phases, 14×14×14 for tetragonal P4₂mc, 13×13×12 for orthorhombic Amm2, 13×13×17 for tetragonal I4₁md. Formation enthalpy (H) for VN is calculated by the equation of

$$\boxed{\times}$$

where the solid molecular N₂ was considered as the chemical potential reference. The hardness of diamond is also calculated to have a comparison.

3. Results and Discussion

3.1 Formation enthalpy and pressure-induced structural phase transition.

In order to obtain a deep insight into the phase stability of VN, the thermodynamic stability of various VN structures as a function of pressure is investigated by the calculation of formation enthalpies. The pressure dependence of the enthalpies is shown in Fig.1. Among the considered structures, VN in the WC structure type is energetically the most stable, in agreement with previous calculated result.^[9] In addition, it is found that at zero pressure the enthalpies of tetragonal P4₂mc, I4₁md and orthorhombic Amm2 phases are all lower than NaCl type phase and exist as new metastable phases. The relative stability order of these considered seven VN structures is WC type > P4₂mc > Amm2 > I4₁md > AsNi type > NaCl type > CsCl type at zero pressure. Such a sequence indicates that WC type has enhanced stability in the considered structures at temperature close to 0 K. The calculations show that VN will undergo a structural phase transition from the WC phase to the CsCl phase as the pressure increases. Two enthalpy curves imply that the WC phase to the CsCl transition occurs at 256 GPa. As far as we know, there are no experimental result available related to the WC-CsCl structural phase transition for comparison. We noticed the transition pressure from NaCl to CsCl phase is about 110 GPa. This result is smaller than 189 GPa from the work of Hao *et al*^[12] due to the difference of calculation method and pseudopotential used.

3.2 The structural properties.

The structural properties are very important for understanding the solid properties from the microscopic viewpoint. Seven structures of VN, e.g. WC, AsNi, NaCl, CsCl,

P4₂mc, Amm2, and I4₁md phases, are simulated using the first-principles calculations. The calculated structural parameters, elastic constants, formation enthalpies per formula unit ($\Delta H/f.u.$), bulk modulus (B), shear modulus (G), Young's modulus (E), Poisson's ratio(ν), and Debye temperature (Θ_D) are listed in table 1. For the purpose of comparison, one can note that our optimized lattices are in good agreement with the experimental value of 4.133 Å (within 0.5%) for NaCl type structure and close to the previous theoretical data for WC, AsNi and CsCl type phases.^[9] Furthermore, for NaCl type phase, the previous studies gave a bulk modulus of experimental value of 268 GPa and theoretical value of 303 GPa, in excellent agreement with our calculated value of 298 GPa. Our calculated elastic constants are also reasonable compared with the experimental and previous theoretical values, indicating that our calculations are valid and believable. Based on the quasi-harmonic Debye model, we give an estimation of Debye temperature from the average sound velocity. However, for the new predicted three metastable P4₂mc, Amm2, and I4₁md phases, there are no any experimental and theoretical values available as the references to our calculated values. In this work, we found that these three structures have the same bulk modulus and the Debye temperatures of them are all higher than that of the rest structures. We hope our results can be served as a prediction for the future experimental investigations.

3.3 pressure dependence of elastic and thermodynamic properties

The elastic constants of solids provide a link between the mechanical and dynamical behavior of crystals, and give important information concerning the nature of the forces operation in solids. Using the pressure dependence of elastic constants, one can judge the mechanical stability of a crystal under high pressure. The Born mechanical stability criteria for hexagonal, cubic, tetragonal, and orthorhombic crystal are given below:^[22]

Hexagonal phase (C_{11} , C_{12} , C_{13} , C_{33} , C_{44})

$$C_{44} > 0, C_{11} > C_{12}, (C_{11} + 2C_{12})C_{33} > C_{13}^2.$$

Cubic phase (C_{11} , C_{12} , C_{44})

$$C_{11} > 0, C_{44} > 0, C_{11} > |C_{12}|, (C_{11} + 2C_{12}) > 0.$$

Tetragonal phase ($C_{11}, C_{12}, C_{13}, C_{33}, C_{44}, C_{66}$)

$$C_{11} > 0, C_{33} > 0, C_{44} > 0, C_{66} > 0, C_{11} - C_{12} > 0, (C_{11} + C_{33} - 2C_{13}) > 0, \\ (2(C_{11} + 2C_{12}) + C_{33} + 4C_{13}) > 0.$$

Orthorhombic phase ($C_{11}, C_{12}, C_{13}, C_{23}, C_{22}, C_{33}, C_{44}, C_{55}, C_{66}$)

$$C_{ii} > 0 (i = 1-6), C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23}) > 0, (C_{11} + C_{22} - 2C_{12}) > 0, \\ (C_{11} + C_{33} - 2C_{13}) > 0, C_{22} + C_{33} - 2C_{23} > 0.$$

Fig.2 presents the hydrostatic pressure dependence of elastic constants of VN for the considered structures. We found that hexagonal WC and AsNi type VN are satisfied the stability conditions when the pressures increase up to 300 and 250 Gpa, respectively. The two hexagonal phases have the same tendency of the five elastic constants at their stable pressure range. That are $C_{33} > C_{11} > C_{44}$ and $C_{12} > C_{13}$, implying the atomic bonds along the [001] direction between nearest neighbors are stronger than the atomic bonds along the [100] direction. It is obviously that the cubic NaCl type structure is only stable as pressure increases up to 125 Gpa, and the CsCl type VN is stable at least as pressure increases above 256 GPa. Our first-principles calculations have given also the same tendency of the three elastic constants $C_{11} > C_{12} > C_{44}$ for the two cubic VN phases taking into account their stable pressure range. C_{11} is more sensitive to the change of pressure compared to other two elastic constants. The large value of C_{11} reflects the strong covalent bonds between the vanadium *d*-like states and the nitrogen *p*-like states along [100] direction. The elastic constants for tetragonal P4₂mc and I4₁md VN phases increase monotonically with increasing pressure except for C_{44} . While the variation of elastic constant C_{44} decreases gradually with the pressure increasing. For the Amm2 phase, the slopes of C_{11} , C_{22} and C_{33} are higher than C_{55} and C_{66} with the pressure increasing. Thus, the elastic constant C_{44} shows the same changing tendency for P4₂mc and

I4₁md phases. The new predicted three phases are all satisfied the mechanical stable conditions until pressure up to 300 GPa, suggesting that the orthorhombic Amm2 phase of VN are unstable when $P > 300$ GPa. From Fig. 3 it can be seen that the pressure has an important influence on the bulk modulus, shear modulus and Debye temperature. The bulk modulus of seven VN structures increase linearly in the similar slope with pressure increasing, indicating it is difficult to be compressed with pressure. This feature has ever been reported by Hao *et al* for NaCl phase.^[12] The variation of shear modulus in CsCl type is higher than other structures among the considered VN structures with pressure increasing. The variation of Debye temperature has the same tendency of increase with shear modulus, showing that the anisotropic of the different VN structures with the pressure increasing.

A proper description of an anisotropic behavior has an important implication in crystal physics. The shear anisotropic factors provide a measure of the degree of anisotropy in the bonding between atoms in different planes. The anisotropic factors of VN in WC, AsNi, NaCl, CsCl, P4₂mc, Amm2, and I4₁md phases as a function of pressure are plotted in Fig.4. For hexagonal crystal, the elastic anisotropy $\frac{C_{11}-C_{12}}{C_{11}+C_{12}}$, $\frac{C_{11}-C_{33}}{C_{11}+C_{33}}$, and $\frac{C_{44}}{C_{11}}$ can be expressed as $\frac{A_1}{C_{11}}$, $\frac{A_2}{C_{33}}$, $\frac{A_3}{C_{44}}$,^[23] where $\frac{A_1}{C_{11}}$, $\frac{A_2}{C_{33}}$, and $\frac{A_3}{C_{44}}$ are the anisotropies for the compression *p*-wave and two shear *s*-waves, respectively. As shown in Fig.4, $\frac{A_1}{C_{11}}$ has no remarkable change, and the change of $\frac{A_2}{C_{33}}$ and $\frac{A_3}{C_{44}}$ goes the opposite direction for both hexagonal WC and AsNi type VN. A measure of the anisotropy of elasticity is by $A = 2C_{44}/(C_{11} - C_{12})$ for cubic crystals. *A* decreases in NaCl and increases in CsCl type structures with the pressure increasing. For the orthorhombic structures, the anisotropic factors for the shear planes {100}, {010}, and {001} are written as:^[24]

$$A_1 = 4C_{44}/(C_{11} + C_{33} - 2C_{13}), A_2 = 4C_{55}/(C_{22} + C_{33} - 2C_{23}),$$

$$A_3 = 4C_{66}/(C_{11} + C_{22} - 2C_{12}).$$

It is interesting to note that there is little difference between A_1 and A_2 while A_3 increases with pressure for Amm2 phase. The shear anisotropic factors of tetragonal VN for {100} and {001} shear planes are defined as

follows:^[25] $A_1 = 2C_{66} / (C_{11} - C_{12})$, $A_2 = 4C_{44} / (C_{11} + C_{33} - 2C_{13})$. We find that A_2 nearly keep constant and A_1 increases sharply for both tetragonal P4₂mc and I4₁md VN phases with the increasing of pressure.

3.4 Density of states and hardness

The band structure and density of states of the WC type VN are presented in fig.5. The band structure indicates that the WC type VN is metallic. From the DOS of fig.5(b), it is found that strong hybridization between N and V states with the energy position. Furthermore, the bonding and antibonding states are composed of N 2*p* and V 4*d* orbitals. The DOS suggests that the chemical bond between N and V atoms is mainly covalent with partial ionicity and metallic contributions. It can be seen from fig.5 that there is a deep valley E_p at the left of the Fermi level, which is termed as pseudogap. This suggests that not all of the bonding states are filled and electrons above E_p become delocalized.

On the other hand, the prediction of the hardness of VN as superhard material is of great potential interest. The estimation of the hardness of nonmetallic materials has been developed by Mulliken population^[26] in the first-principles techniques. Since the metallic bonding is delocalized and not directly related to hardness. The hardness calculation should be corrected. Here the correction of the hardness for the compound crystals with metallic bonding is expressed as $\frac{M}{M + \nu_b}$, where M is the Mulliken population, ν_b is the metallic population, and ν_b is the volume of the bond. The metallicity of crystals can be defined as $\frac{\nu_b}{M + \nu_b}$. Calculated hardness of VN in various structures and diamond are listed in Table 2. The metallicity of VN in NaCl type VN structure is 0.46, and its hardness is 17.1GPa, which are in good agreement with the experimental results^[27] and the previous theoretical results.^[29] Otherwise, the calculated hardness of diamond is 97.8 GPa, in excellent consistent with experimental 100 GPa, indicating our calculations are reliable. The hardnesses of Amm2, and I4₁md structures are 19.5, 28.8 and 19.8 GPa, respectively, which are higher than WC, AsNi and NaCl type VN structures. When we

take Jiang's empirical formula ^[30] to evaluate the hardness values of VN in various structures according to the bulk modulus and shear modulus, we found the Mulliken population method are more close to experimental values to evaluate the hardness of metallic bonding compounds. We hope our work should be useful for understanding the effect of metallic bonding on the hardness of VN in various structures.

4. Conclusions

In summary, according to above investigation, we have the following conclusions:

- 1) It is predicted that the tetragonal $P4_2mc$, $I4_1md$, and orthorhombic $Amm2$ phases of VN are energetically more stable than NaCl type structure. Together with WC, CsCl, NaCl, and AsNi phases, we found that the phase transition from WC to CsCl structure occurs at 256 GPa. The further experimental investigations may be required to clarify the new predicted phases and the WC-CsCl structural phase transition.
- 2) The structural parameters, elastic and thermodynamic properties of VN in various structures have been derived. It is found that the Debye temperatures of $P4_2mc$, $Amm2$, and $I4_1md$ phases are all higher than other structures. The hexagonal WC and AsNi type VN are mechanical stable at pressures up to 300 and 250 Gpa, respectively. The cubic NaCl type is only stable as pressure increases up to 125 Gpa, and the CsCl type VN is stable at pressures above 256 GPa. The predicted three new phases are all stable until pressure increases up to 300 GPa based on the mechanical stable criteria.
- 3) The calculated result of the electronic structure and density of states of WC type indicate that VN is metallic. The bonding nature of N and V are strong hybridized as covalent. The calculation on the hardness of VN in various structures indicates that the hardnesses of $Amm2$, and $I4_1md$ structures are 19.5, 28.8 and 19.8 GPa, respectively.

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Table and Figure Captions

TABLE 1. The calculated lattice constants, a_0 (Å), c_0 (Å), cell volume per formula unit (Å³), and formation enthalpy per formula unit ΔH (eV), bulk modulus B (Gpa), shear modulus G (Gpa), Yong's modulus E (Gpa), Poisson's ratio ν , and Debye temperature Θ_D (K) at the Norm-conserving pseudopotential method for VN from various space groups: hexagonal (WC type, P-6M2, No. 187; AsNi type, P63/mmc, No. 194), cubic (NaCl type, Fm-3m, No. 225; CsCl type, Pm-3m, No. 221), tetragonal (P4₂mc, No. 105; I4₁md, No. 109), and orthorhombic (Amm2, No. 38) phases.

TABLE 2. Calculated hardness of VN in WC, CsCl, NaCl, AsNi, P4₂mc, Amm2, and I4₁md structures and diamond. Structure data were taken from the results of GGA of Ultrasoft pseudopotential method, where H_{vcal} (Gpa) and H_{vexp} (Gpa) are the calculated and experimental hardness, respectively.

FIG 1. (color online) Enthalpy as a function of pressure for VN in WC, CsCl, NaCl, AsNi, P4₂mc, Amm2, and I4₁md structures at T=0K.

FIG 2. (color online) Pressure dependence of elastic constants in (a) WC type, (b) AsNi type, (c) NaCl type, (d) CsCl type, (e) P4₂mc, (f) I4₁md, and (g) Amm2 structures of VN.

FIG 3. (color online) Pressure dependence of the bulk modulus B (Gpa), shear modulus G (Gpa) and Debye temperature Θ_D (K) in WC, CsCl, NaCl, AsNi, P4₂mc, Amm2, and I4₁md structures of VN.

FIG 4. (color online) Pressure dependence of the anisotropic factors in WC, CsCl, NaCl, AsNi, P4₂mc, Amm2, and I4₁md structures of VN.

FIG 5. (color online) (a) Band structure. (b) DOS and PDOS of WC-VN

Table 1

	WC	NaCl	CsCl	AsNi	P4 ₂ mc	Amm2	I41md
a (Å)	2.763	4.153, 4.133 ^a , 4.13 ^b	2.562	2.793	2.699	2.716	2.699
b (Å)						2.684	
c (Å)	2.656			5.204	9.611	14.424	9.622
ΔH (eV)	-2.259	-1.833, -2.0 ^c	-1.161	-2.059	-2.221	-2.220	-2.215
Volume (Å ³)	17.552	17.902	16.807	17.582	17.515	17.524	17.528
C_{11}	550	514, 591 ^b , 533 ^d	846	540	708	675	712
C_{22}						746	
C_{33}	810			676	572	582	585
C_{44}	250	108, 137 ^b , 133 ^d	140	179	216	226	219
C_{55}						206	
C_{66}						264	
C_{12}	184	189, 159 ^b , 135 ^d	13	180	128	128	131
C_{13}	129			143	138	138	130
C_{23}						131	
B	308	298, 303 ^b , 268 ^d	291	298	310	310	310
G	229	128, 164 ^b	221	192	243	243	247
E	551	336, 417 ^b	529	474	578	578	586
ν	0.202	0.312, 0.270 ^b	0.197	0.235	0.189	0.189	0.185
Θ_D	974	739	949	894	1001	1002	1009

^aReference 18^bReference 19^cReference 20^dReference 21**Table 2**

	d (Å)	P	P'	f_m	ν_b (Å ³)	H_{vcal}	H_{vexp}
Diamond	1.544	0.750			2.835	97.8	100.6 ^a
WC	2.064	0.265	0.118	0.45	2.873	18.7	
NaCl	2.060	0.262	0.121	0.46	2.913	17.1	16 ^b
CsCl	2.203	0.197	0.030	0.15	2.058	37.1	
AsNi	2.056	0.257	0.116	0.28	2.861	18.1	
P4 ₂ mc	2.056	0.265	0.113	0.43	2.869	19.5	
Amm2	2.091	0.310	0.115	0.37	2.583	28.8	
I41md	2.088	0.270	0.115	0.43	2.869	19.8	

^aReference 27^bReference 28

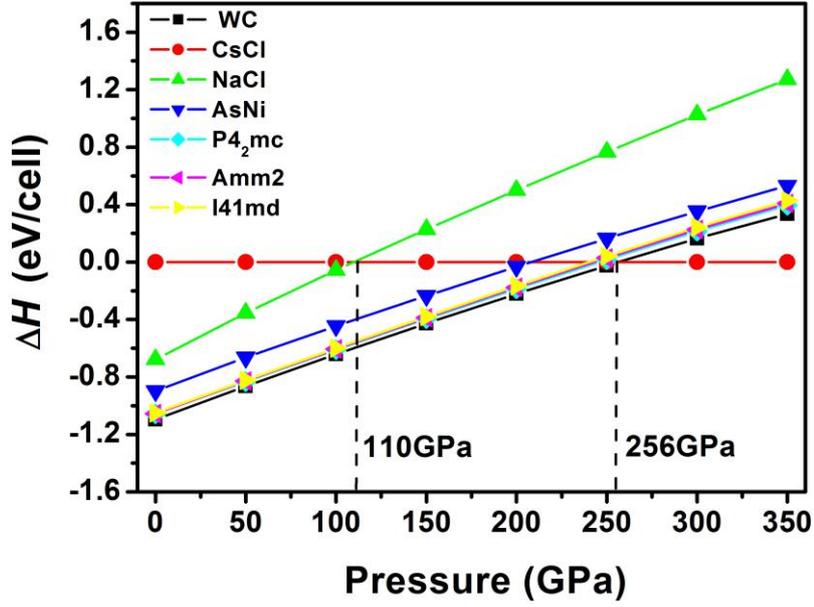
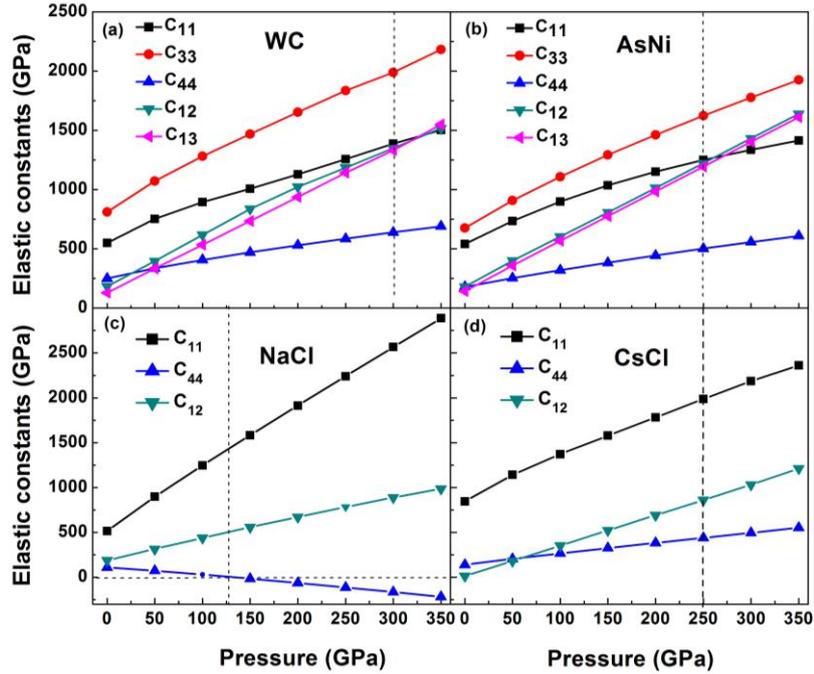


Fig. 1



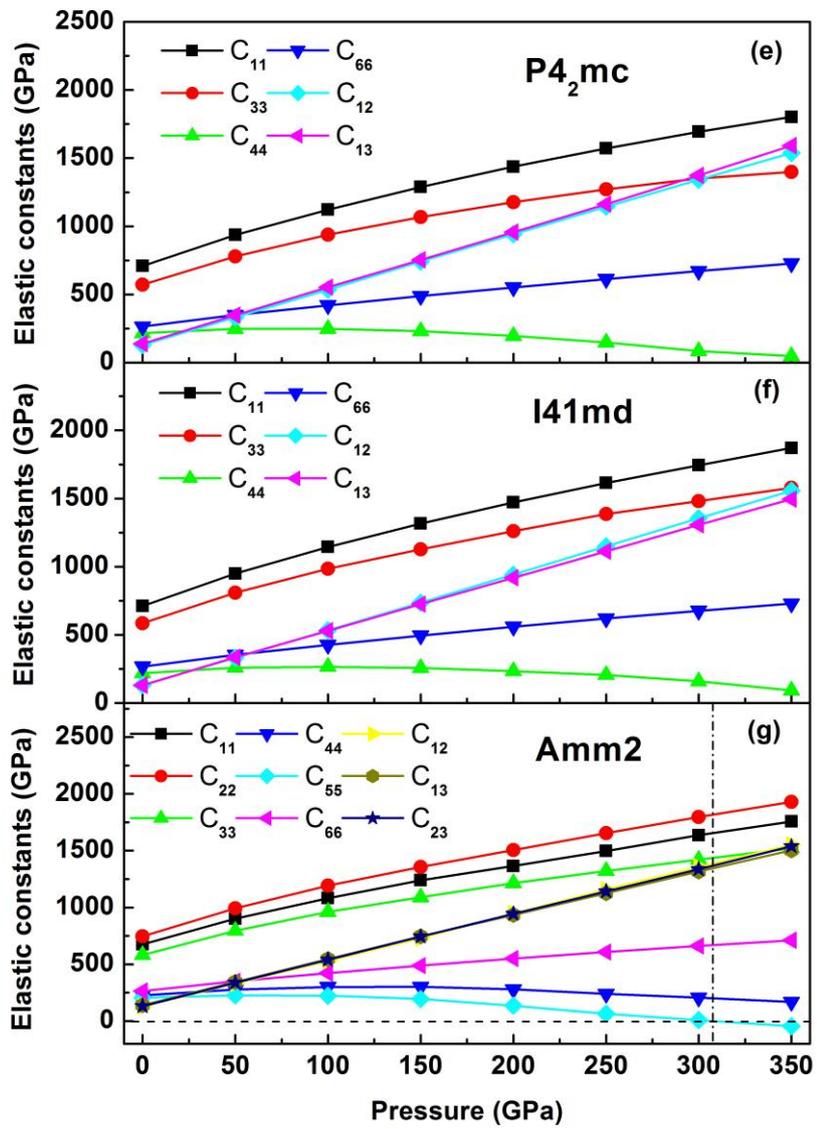


Fig. 2

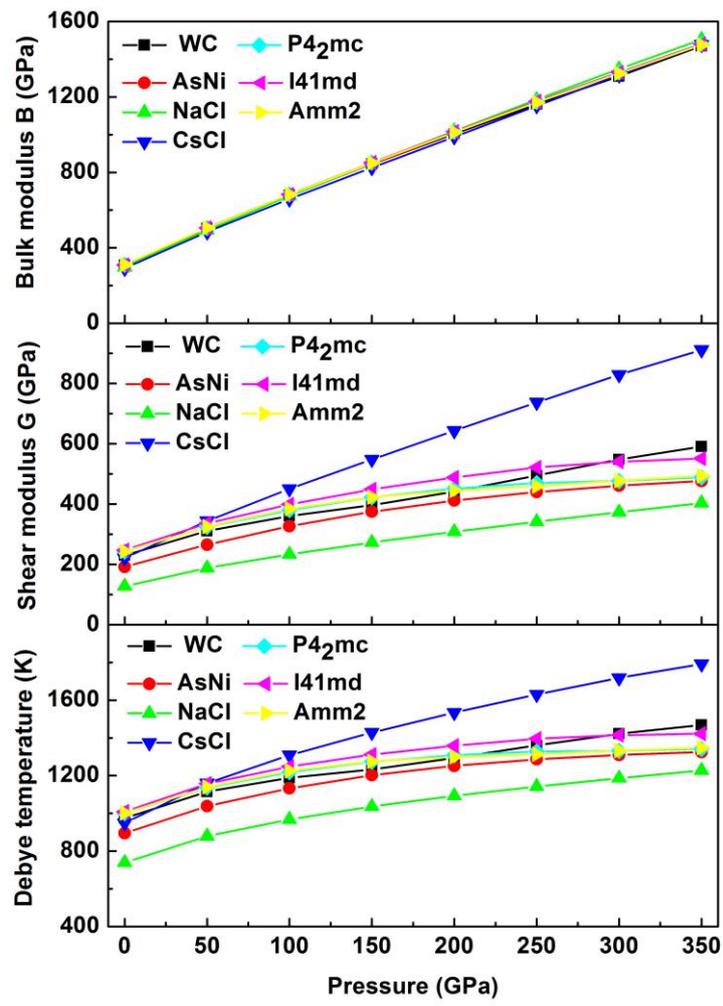


Fig. 3

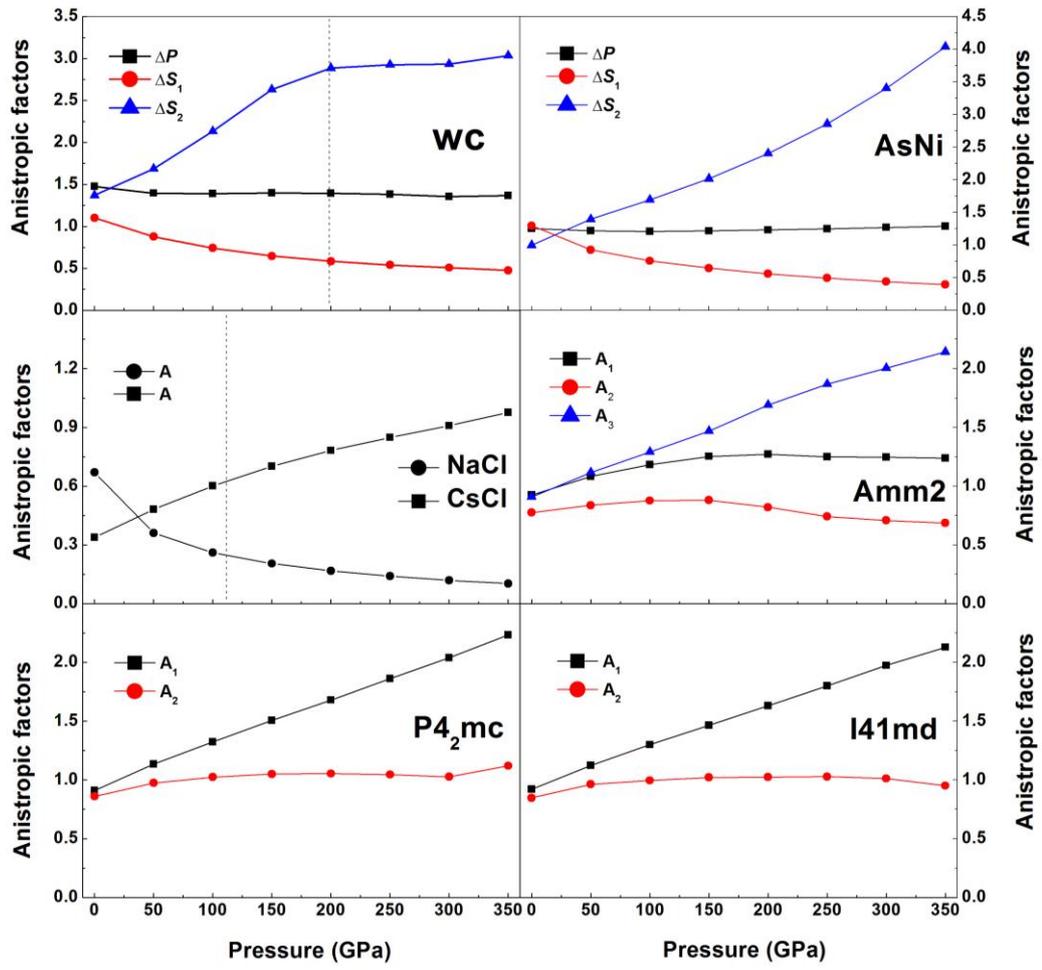
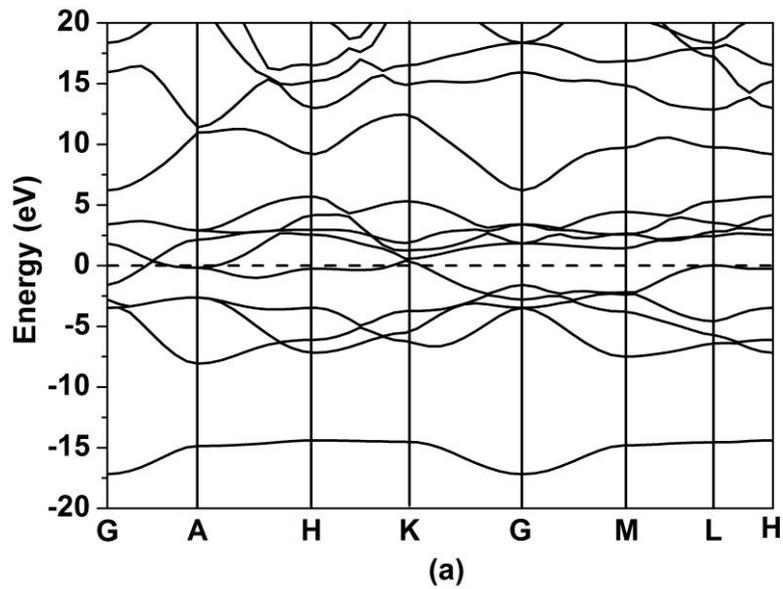


Fig.4



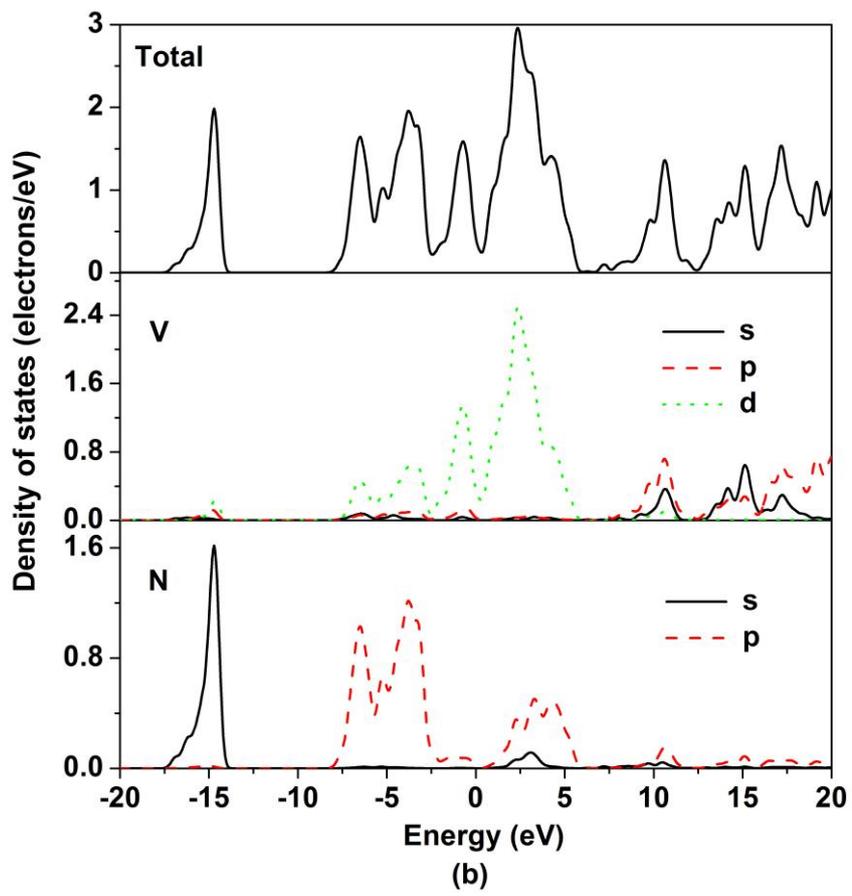


Fig. 5