Advances in Physics Theories and Applications
ISSN 2224-719X (Paper) ISSN 2225-0638 (Online)
Vol.19, 2013 - Selected from International Conference on Recent Trends in Applied Sciences with Engineering Applications
www.iiste.org

High Pressure Study of IrN in Zinc-Blende Structure

Madhu Sarwan (Corresponding author)
Department of Physics, Barkatullah University, Bhopal, India 462026
E-mail: madhusarwan@gmail.com
Bashir Ahmed Mir, Faisal Shareef M, Vasudev Thakre and Sadhna Singh
Department of Physics, Barkatullah University, Bhopal, India 462026
E-mail: drsadhna100@gmail.com

Abstract

The structural phase transition, volume collapse and second order elastic constants of 5d-transition metal mononitride (IrN) have been investigated by using interaction potential model (IPM) which consists of Coulomb interaction, three-body interaction and short range overlap repulsive interactions. The present theoretical approach has predicted pressure-volume relationship curves which shows that IrN exhibits a zinc-blend (ZB) type structure at an ambient pressure and undergoes a structural phase transition from B3 to B1 phase at pressure 72 GPa. The equation of state shows volume collapse of 9.09 %. The phase transition pressure and associated volume collapses obtained from this model show a reasonable agreement with other theoretical results. The second order elastic constants are also investigated for ZB phase.

Keywords: High Pressure, Phase Transition, Transition Metal Compounds

1. Introduction

Transition metal nitrides have received much attention from experimental and theoretical workers in recent years because of their excellent properties such as hardness, superconductivity, photoluminescence and various type of magnetism [1]. The iridium mononitride (IrN) compound is the least studied among the family of these transition metal nitrides. Rached et.al. [2] investigated the elastic, structural and electronic properties of IrN by using first-principle calculation. The nature of interatomic forces is not well understood in these compounds and phenomenological model based on various interatomic interaction energies to determine stable structure becomes important. In the present study, we have applied an interaction potential model (IPM) to study high pressure phase transition and elastic properties. In the present model we have included three-body interaction (TBI) forces [3-5]. This TBI approach has been extended to include the Hafemeister-Flygare (HF) type [6] overlap repulsion operative up to the second neighbour ions.

2. Present Potential Model

The application of pressure on the crystal causes the decrease in their volume, which in turn leads to an increased charge transfer (or exchange) between the overlapping electron shells of the adjacent ions. This transferred charge modifies the ionic charge which when interacts with other distant charges gives rise to many body interactions (MBI), the dominant part of MBI is three-body interactions [3].

These TBP effects have been incorporated in the Gibbs free energy (G=U+PV-TS). Here, U is the internal energy which at T=0K is equivalent to the lattice energy, S is the vibrational entropy at absolute temperature T. At T=0K and pressure P, the Gibbs free energy for the zinc-blend (B3, real) and NaCl (B1, hypothetical) structures are given by

$$G_{B3}(r) = U_{B3}(r) + PV_{B3} \qquad (1)$$

$$G_{B1}(r') = U_{B1}(r') + PV_{B1} \qquad (2)$$

With V_{B3} (3.08 r^3) and V_{B1} (2.00 r'^3) as unit cell volumes for B_3 and B_1 phases, respectively. The first term in (1) and (2) are lattice energies for B_3 and B_1 structures and they are expressed as

$$U_{B3}(r) = \frac{-\alpha_M e^2 Z^2}{r} - \frac{4\alpha_M e^2 Zf(r)}{r} + 4b\beta_{ij}\exp(r_i + r_j - r_{ij}/\rho) \qquad (3)$$

$$U_{B1}(r) = \frac{-\alpha'_M e^2 Z^2}{r'} - \frac{6\alpha'_M e^2 Zf(r)}{r'} + 6b\beta_{ij}\exp(r_i + r_j - r'_{ij}/\rho) \qquad (4)$$

With α_M and α'_M as the Madelung constants for ZnS and NaCl structures, respectively. β_{ij} (i,j = 1,2) are the Pauling coefficients defined as $\beta_{ij} = 1 + (Z_i/n_i) + (Z_j/n_j)$ with Z_i (Z_j) and n_i (n_j) as the valence and the number of electrons of the i (j)th ion. Ze is the ionic charge and b (ρ) are the hardness (range) parameters, r(r') are the nearest neighbour separation for ZnS (NaCl) structure. f(r) is the three-body force parameter r_i (r_j) are the ionic radii of ions i (j). These lattice energies consist of long range Coulomb energy (first term), three-body interactions corresponding to the nearest neighbour separation r (r') (second term), energy due to the overlap repulsion represented by Hafemeister and Flygare (HF) type potential (third term).

3. Result and Discussions

The present interaction potential model (IPM) contains three model parameters b, ρ and f(r), namely hardness, range and three-body interaction parameter. These parameters are calculated by using the first derivative of cohesive energy (U) and equilibrium condition expressed as:

$$\left|\frac{dU}{dr}\right|_{r=r0} = 0 \qquad (5)$$

$$B1+B2=-1.261Z[Z+8f(r)] \qquad (6)$$

The input data and model parameters are given in table 1. As the stable phase is always associated with minimum of energy, we have minimized G_{B3} (r) and G_{B1} (r') at different pressures in order to obtain inter ionic separations r and r' for B3 and B1 phases respectively associated with minimum energies.

We have evaluated the corresponding G_{B3} (r) and G_{B1} (r') and their respective differences $\Delta G=G_{B3}(r)-G_{B1}(r')$. A positive value of ΔG at zero pressure justifies the stability of B3 phase. As the pressure is increased the value of ΔG decreases and approaches to zero at the transition pressure (P_t). Beyond this pressure ΔG becomes negative as the phase B1 become stable. The Gibb's free energy difference $\Delta G = G_{B3}(r)-G_{B1}(r')$ has been plotted as a function of pressure (P) in Fig. 1. The pressure corresponding to ΔG approaching zero is the phase transition pressure (P_t). The phase transition pressures so obtained are presented in Table 2 along with the other theoretical results [1]. Fig. 1 shows the phase transition from ZB to RS structure in IrN at 72 GPa. The phase transition pressure is illustrated by arrow in Fig. 1.

Under pressures, the materials transform from one structure to another structure with a sudden change in arrangement of atoms. These atoms are rearranged in new position and give rise to the new structure. Experimentally one usually studies the relative volume change associated with compressions. The discontinuity in volume at the transition pressure is obtained from the phase diagram. The values of relative volume associated with various compressions have been computed by using the interaction potential model. Deduced the pressure dependent radii r and r' for both the structures (B3 and B1) have been used to compute the relative volume changes and are plotted against the pressure (P) in Fig. 2. The magnitude of the discontinuity in volume change at the transition pressure has been obtained from the phase diagram and the value is listed in Table 2.

The elastic constants are important properties of solids which provide a link between the mechanical and dynamic behaviors of crystals. They provide information on the elasticity, stability and stiffness of crystals and give important information about nature of forces operating in solids. While studying the high pressure elastic behavior of IrN we have computed the second order elastic constants (SOECs) C_{11}, C_{12} and C_{44} as they provide physical insight into the nature of binding forces between different constituents of a crystal. In the present model we have included three body interaction forces. The inclusion of three body interaction forces was emphasized by Sims et al. [7]. Earlier calculations were based on two-body potential mainly. They concluded that possible reasons for disagreements include the failure of the two body potential model. Since these studies were based on two body potentials and could not explain Cauchy violations $C_{12} \neq C_{44}$. Our model is able to explain Cauchy violation $C_{12} \neq C_{44}$ in second order elastic constants. One common approach is to assume that the atoms are connected with springs and that the resulting forces are only in the direction of the nearest neighbours (central force model). The deviation from the Cauchy violation $\delta=C_{12}-C_{44}-2P$ is a measure of the contribution from the non central many-body force. Our calculations give negative $C_{12}-C_{44}$ values (Table 3). $C_{44}>C_{12}$ inequality is observed in the present work.

The method for their calculations is same which we have reported in our earlier work [4]. The values of SOECs are given in Table 2. We note that the values of C_{11}, C_{12} and C_{44} are better matching with others [1].

4. Conclusion

We have applied interaction potential model (IPM)) to investigate the structural phase transition and elastic properties of IrN compounds. An overall assessment shows that, our values of IPM near to available are in general matching with other theoretical results. Our results where no experimental results are available may be tested with different theoretical and experimental methods in future.

Acknowledgement
The authors are thankful to the U.G.C.(SAP) New Delhi for the financial support.

References

[1] Chen W. and Jiang J. Z. (2010) Elastic properties and electronic structures of 4d and 5d transition metal mononitrides, J. of Alloys and compounds, 499, 243.
[2] Rached H, Rached D, Khenata R, Benalia S, Rabah M, Semari F and Righi H (2011) Structural stabilities, elastic and electronicmononitride: A first-principles study, Phase Transitions, 84, 269-283.
[3] Singh R. K. (1982) Many body interactions in binary ionic solids, Phys Rep. 85, 259-401.
[4] Singh R.K. and Singh S. (1989) Structural phase transition and high pressure elastic behavior of III-V semiconductors, Phys. Rev. B, 39, 671-676.
[5] Bhardwaj P., Singh S. and Gaur N. K. (2009) Structural, elastic and thermophysical properties of divalent metal oxides with NaCl structure, Mater. Res. Bull., 44, 1366-1374.
[6] Hafemiester D. W. and Flygare H. F. (1965) J. Chem. Phys. 43, 795.
[7] Sims C. E., Barrera G. D. and Allan N. L. (1998) Thermodynamics and mechanism of the B1- B2 phase transitionin group-I hailides and group-II oxides, Phys. Rev. B, 57, 11164-11172.

Table 1 Input and model parameters of IrN.

Input parameters			Model parameters		
r_1 (Å)	r_2(Å)	a(Å)	b(10^{-12} ergs)	ρ (Å)	f(r)
0.82	1.47	4.64[1]	0.8297	0.402	-0.0962

Table 2 Input and model parameters of IrN.

	Phase transition Pressure (GPa)	Volume collapse (%)	Elastic constants (GPa)		
			C_{11}	C_{12}	C_{44}
IPM	72	9.09	326.54	213.09	50
Exp.	-	-	-	-	-
Other [1]	72		322	256	34

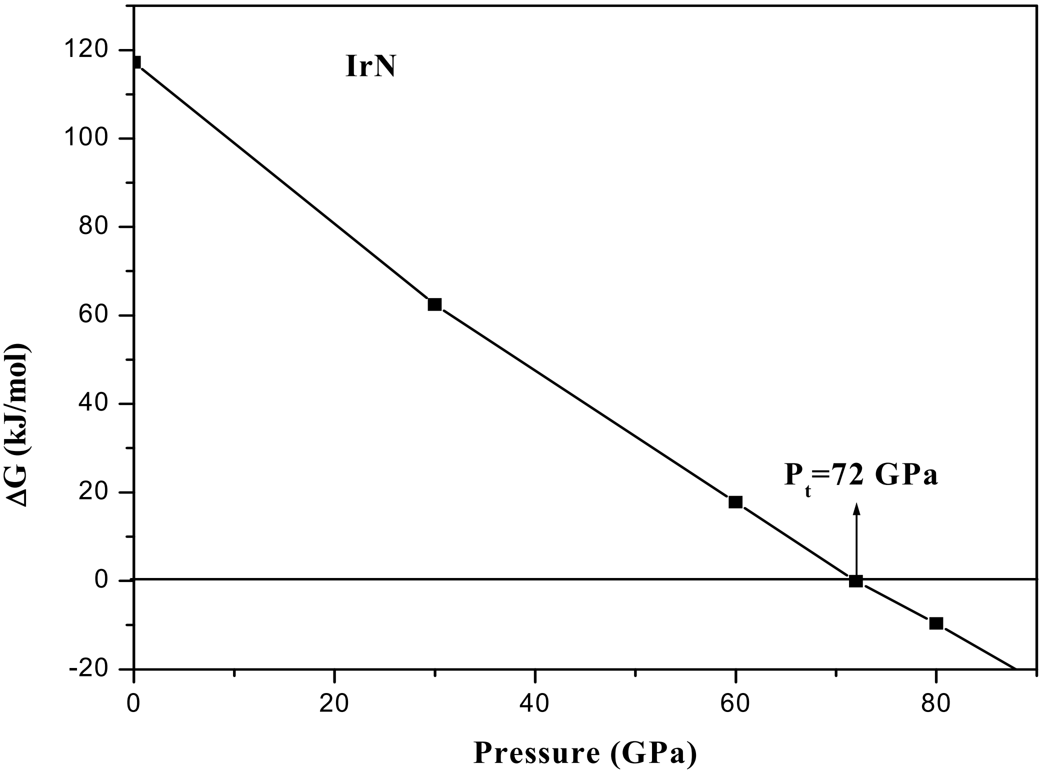

Fig. 1 Variation of change in Gibbs free energy with pressure.

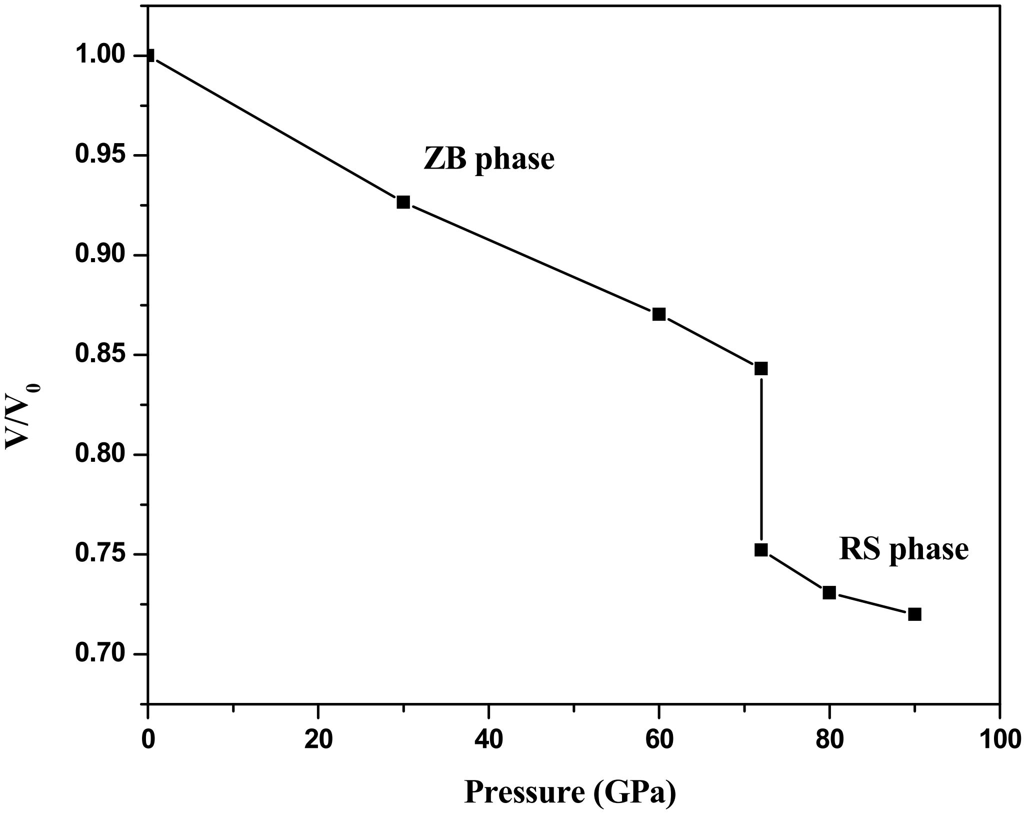

Fig. 2 Variation of V/V_0 with pressure.

This academic article was published by The International Institute for Science, Technology and Education (IISTE). The IISTE is a pioneer in the Open Access Publishing service based in the U.S. and Europe. The aim of the institute is Accelerating Global Knowledge Sharing.

More information about the publisher can be found in the IISTE's homepage:
http://www.iiste.org

CALL FOR PAPERS

The IISTE is currently hosting more than 30 peer-reviewed academic journals and collaborating with academic institutions around the world. There's no deadline for submission. **Prospective authors of IISTE journals can find the submission instruction on the following page:** http://www.iiste.org/Journals/

The IISTE editorial team promises to the review and publish all the qualified submissions in a **fast** manner. All the journals articles are available online to the readers all over the world without financial, legal, or technical barriers other than those inseparable from gaining access to the internet itself. Printed version of the journals is also available upon request of readers and authors.

IISTE Knowledge Sharing Partners

EBSCO, Index Copernicus, Ulrich's Periodicals Directory, JournalTOCS, PKP Open Archives Harvester, Bielefeld Academic Search Engine, Elektronische Zeitschriftenbibliothek EZB, Open J-Gate, OCLC WorldCat, Universe Digtial Library , NewJour, Google Scholar