Journal of the Association of Arab Universities for Basic and Applied Sciences (2013) **14**, 38–45

University of Bahrain
Journal of the Association of Arab Universities for Basic and Applied Sciences
www.elsevier.com/locate/jaaubas
www.sciencedirect.com

حساب الضغط ومعامل المرونة الحجمي للهاليدات القلوية عند الضغط العالي ودرجات الحرارة العالية باستخدام معادلات الحالة المختلفة

ابتسام يحيى عبدالله الكماش

قسم الفيزياء، كلية العلوم، جامعة الموصل، العراق

الملخص:

تم في هذا البحث استخدام معادلات الحالة الغير المقلوبة (الايزوثرمية) والتي تعتمد أساسا على الجهد بين الأيونات مثل: معادلة حالة (فنت– ريدبرج) ومعادلة حالة شانكير ومعادلة حالة باردين وأخيرا معادلة حالة كومر الايزوثرمية، وذلك لدراسة تغير الانضغاطية الحجمية النسبية في مدى 1–0.5 ومعامل المرونة الحجمي الايزوثرمي مع الضغط عند درجة حرارة 300K لأربعة هاليدات قلوية (NaF, NaCl, NaBr, NaI). ولقد تم أيضا مقارنة نتائج الإنضغاطية النسبية التي تم الحصول عليها من معادلات الحالة الأربعة مع النتائج التجريبية والتي بينت أن جميع النتائج أظهرت توافقا جيدا عند ضغط يقدر بـ 15GPa. أما عند ضغوط أعلى من ذلك فكانت نتائج معادلة حالة (فنت – ريدبرج) ومعادلة حالة شانكير ومعادلة حالة باردين والنتائج التجريبية متوافقة في هذا المدى الواسع من الضغط. ولكن نتائج معادلة حالة كومر الايزوثرمية عند الضغط العالي فقد انحرفت عن معادلات الحاله الأخرى. وعلى كل حال، فلقد بينت نتائج الإنضغاطية الايزوثرمية عندما تكون الإنضغاطية الحجمية النسبية تساوي 0.5 فأن الضغوط العالية المحسوبه هي 170GPa، 90GPa و 60GPa للهاليدات القلوية NaF و NaCl و NaBr و NaI على الترتيب.

وكذلك تم مقارنة نتائج معامل المرونة الحجمي الايزوثرمي (K_T) التي تم الحصول عليها من معادلات الحالة الأربعة وتبين أن معامل المرونة يزداد باستمرار بزيادة الضغط ولقد أظهرت النتائج تطابقها عند ضغط مقداره 1GPa ولكن أعلى من ذلك فأن النتائج تحيد بعضها عن الاخر لمعادلات الحالة الأربع.

وأخيرا، تم دراسة تغير الإنضغاطية الحجمية النسبية ومعامل المرونة الحجمي غير الايزوثرمي مع الضغط العالي باستخدام معادلة حالة كومر الغير الايزوثرمية العامة.

Journal of the Association of Arab Universities for Basic and Applied Sciences (2013) **14**, 38–45

University of Bahrain

Journal of the Association of Arab Universities for Basic and Applied Sciences

www.elsevier.com/locate/jaaubas
www.sciencedirect.com

ORIGINAL ARTICLE

Evaluation of pressure and bulk modulus for alkali halides under high pressure and temperature using different EOS

Ibtisam Y. Alkammash

Department of Physics, College of Science, University of Mosul, Iraq

Received 3 August 2012; revised 20 November 2012; accepted 5 January 2013
Available online 21 February 2013

KEYWORDS

Equation of state;
Kumar General EOS;
Interionic potential;
Compressibility;
Bulk modulus;
Alkali halides

Abstract In the present work, the non-inverted (isothermal) type equations of state (EOS) which are based on interionic potential such as Vinet–Rydberg EOS, Shanker EOS, Bardeen EOS as well as Kumar isothermal EOS are used to study the variation of relative compression volumes in range 1–0.5 and the isothermal bulk modulus with high pressure at temperature $T = 300$ K for four alkali halides (NaF, NaCl, NaBr and NaI).

The results for relative compression volume obtained from the four EOS have been compared with experimental data which indicated that up to 15 GPa they are in good agreement. But beyond this, the results which have been obtained from the Vinet–Rydberg EOS Shanker EOS and Bardeen EOS as well as from the experimental data showed that they are also in good agreement in the wide range of high pressure. While results obtained from Kumar isothermal EOS showed that beyond 15 GPa they deviated from the other EOS. Moreover the results of isothermal compressibility have shown that at the value 0.5, the calculated high pressures are equal to (170, 90, 78 and 60) GPa for NaF, NaCl, NaBr and NaI respectively.

The results for the isothermal bulk modulus (K_T) have been compared with four EOS and showed that the bulk modulus increases continuously with increase in pressure. The results indicated that up to 1 GPa are found to be in good convergence, but beyond this range, the results do diverge from each other for the four EOS.

Finally, the variations of non-isothermal compression (inverted) and non-isothermal bulk modulus with high pressure have been investigated by using a non-isothermal Kumar EOS (Kumar General EOS).

1. Introduction

The understanding of the ionic solids at nonambient conditions is an integral part of the work of material scientists, solid state physicists, chemists, and solid earth geoscientists that are routinely confronted with problems involving ionic solids at high pressure and high temperature (Anderson, 1995).

The EOS play a central role in the study of the material. These equations describe the relationships between the

E-mail address: ibtisamyahya@yahoo.com

Peer review under responsibility of University of Bahrain.

ELSEVIER Production and hosting by Elsevier

http://dx.doi.org/10.1016/j.jaubas.2013.01.001

pressure, temperature and volume (Kushwah et al., 2007) and (Kushwah and Bhardwaj, 2009). Using the EOS, some important properties such as compressibility of solid can be calculated. In addition, the EOS enable one to determine the depth dependence of important thermoelastic parameters, such as thermal expansivity and temperature sensitivity of bulk modulus.

The theoretical attempt for obtaining EOS may be divided mainly into two categories (Anderson, 1995) (i) interionic potential based model (ii) interionic potential independent models. However, it has been observed that the methods based on the theory of interionic potential are difficult to deal with (Singh et al., 1991) and not even be possible to realize in some complicated solids like minerals. On the other hand the second one is free from these difficulties. A theoretical study based on potential model was performed by Sun (Sun, 2007). He obtained bulk modulus results that are in good agreement with the Vinet–Rydberg EOS. A potential independent model was developed by Sharma (Sharma et al., 2010) for C_{60} solid under varying conditions of pressure and temperature.

The aim of this work is to study some thermodynamical properties of some alkali halides (NaF, NaCl, NaBr and NaI) under high pressure using the non-inverted (isothermal) equation of state based on interionic potential such as Vinet–Rydberg EOS, Shanker EOS, Bardeen and Kumar EOS. In order to achieve this study, the theoretical calculation for compressibility and bulk modulus must be done at different high pressures and at 300 K. The calculation results will be compared with experimental data obtained from Sorensen (Sorensen, 1983). Moreover, the variation of compressibility and bulk modulus versus pressure at different temperatures will be investigated using the inverted (non-isothermal) Kumar General EOS for alkali halides.

2. Theory

2.1. Preamble

The pressure–volume (P–V) relationship for a solid at a given temperature can be expressed as non-inverted type as given in Eq. (1), or as inverted type as given in Eq. (2) (Digpratap et al., 2007)

$$P = f\left(\frac{v}{v_0}, K_0, K_0', K_0''\right) \tag{1}$$

$$\frac{v}{v_0} = f(P, K_0, K_0', K_0'') \tag{2}$$

where V_o is the volume at pressure $P = 0$. K_0, K_0' and K_0'' are the values of bulk modulus, first pressure derivatives and second pressure derivatives respectively, all at $P = 0$.

Equation of state for inverted and non-inverted types for solids is derived from the relation (Tosi, 1964):

$$P = -\frac{dE}{dV} \tag{3}$$

where E is the interionic potential energy and V is the volume

The bulk modulus (K_T) for inverted and non-inverted types can be derived from the following equation:

$$K_T = -V\frac{dP}{dV} \tag{4}$$

2.2. Non-Inverted Type EOS

During the last years, many researchers have used Birch-Murnghan EOS as the non-inverted type (isothermal) in the field of solid state physics and geophysics ((Digpratap et al., 2007). This EOS is based on the Eulerien finite strain theory (Birch, 1952). But recent studies (Hama and Suito, 1996), (Poirier and Tarantola, 1998), (Shanker et al., 1999) and (Sushil et al., 2004) reveal that Birch-Murnghan EOS does not describe adequately the compression of the solid at high pressures. However, the following EOS have been found to be the best way to describe adequately the compression of solids at high pressure.

2.2.1. Vinet–Rydberg (V–R) EOS

One of the most successful isothermal EOS is that proposed by Vinet et al. (Vinet et al., 1986) and (Vinet et al., 1986) which is valid for all classes of solids in compression and in the absence of phase transition. The basis of this EOS is a universal relation for the binding energy in terms of the interionic distance. In the derivation of this EOS contribution of the thermal pressure is neglected, and the volume derivative of the binding energy is used to approximate the internal energy.

The Vinet EOS based on the Rydberg potential function has been widely used in spite of its main shortcoming regarding the extreme compression behavior of solids. Vinet–Rydberg have obtained an EOS which is based on the Rydberg potential energy $E(r)$ expressed as a function of the interionic distance (r) (Rydberg,1932).

$$E(r) = E(a)[1 - b\left(1 - \frac{r}{a}\right)\exp b\left(1 - \frac{r}{a}\right) \tag{5}$$

where a and b are the potential parameters.

The (V–R) EOS is written as (Vinet et al., 1989):

$$P = 3K_0x^{-2/3}(1 - x^{1/3})\exp[\eta(1 - x^{1/3})] \tag{6}$$

where $x = V/V_o$ and $\eta = \frac{3}{2}(K_0' - 1)$

The isothermal bulk modulus can be written as:

$$K_T = K_0x^{-2/3}[1 + \{\eta x^{1/3} + 1\}(1 - x^{1/3})]\exp[\eta(1 - x^{1/3})] \tag{7}$$

2.2.2. Shanker EOS

Owing to the fact that the pressure and the isothermal bulk modulus may be expressed as a function of the lattice potential energy, and also the derivatives of potential energy with respect to volume may be expressed in terms of the derivatives of (E) with respect to the interionic distance (r), Shanker (Shanker et al., 1997) and (Shanker et al., 1999) introduced a force constant (F) in terms of Laplacian operator (Born and Huang, 1954), and he found that F may be expressed as a function of volume mentioned in references Shanker (Shanker et al., 1997) and (Shanker et al., 1999) then with some mathematical manipulation he obtained a result known as Shanker EOS.

Shanker et al. have obtained an EOS using the volume dependence of the short-range force constant for interionic potentials. The short range force constant (F) is defined as follows:

$$F = \frac{1}{3}\left(\frac{d^2E}{dr^2} + \frac{2}{r}\frac{dE}{dr}\right) \tag{8}$$

Table 1 Values of input parameters used in the present work.

	NaF	NaCl	NaBr	NaI
K_o(GPa)	46.5	24.0	19.9	15.1
K'_0	5.28	5.39	5.49	5.59
α0 × 10–4(K-1)	0.96	1.19	1.26	1.37
δ_{T_0}	5.77	5.85	6.23	6.43

The expression based on the Shanker EOS is given below (Shanker et al., 1997 and (Shanker et al.,1999).

$$P = K_0 \frac{x^{-4/3}}{t}\left[\left(1+\frac{1}{t}+\frac{2}{t^2}\right)\{\exp(ty)-1\}+y\left(1+y-\frac{2}{t}\right)\exp(ty)\right] \tag{9}$$

where $x = V/V_o, t = K'_0 - \frac{8}{3}$ and $y = 1-(V/V_o)$.

The isothermal bulk modulus can be written as:

$$K_T = K_0 x^{-1/3}(1+y+y^2)\exp(ty)+\frac{4}{3}P \tag{10}$$

where $x = V/V_o, t = K'_0 - \frac{8}{3}$ and $y = 1-(V/V_o)$.

2.2.3. Bardeen EOS

The Bardeen equation of state is derived from the potential function $E(r)$ (Bardeen, 1938):

$$E(r) = \frac{a}{r^3}+\frac{b}{r^2}-\frac{c}{r} \tag{11}$$

where a, b and c are constants.

The Bardeen EOS is written as (Butler and Anderson, 1978):

$$P = 3K_0[x^{-5/3}-x^{-4/3}]\left[1+\frac{3}{2}(K'_0-3)(x^{-1/3}-1)\right] \tag{12}$$

where $x = V/V_0$

The isothermal bulk modulus (K_T) has been derived by (author), using Eq. (4).

$$K_T = -\left(\frac{-5}{3}x^{-5/3}+\frac{4}{3}x^{-4/3}\right)\left(1+\frac{3}{2}(K'_0-3)(x^{-1/3}-1)\right) + K_0(x^{-5/3}-x^{-4/3})\frac{3}{2}(K'_0-3)x^{-1/3} \tag{13}$$

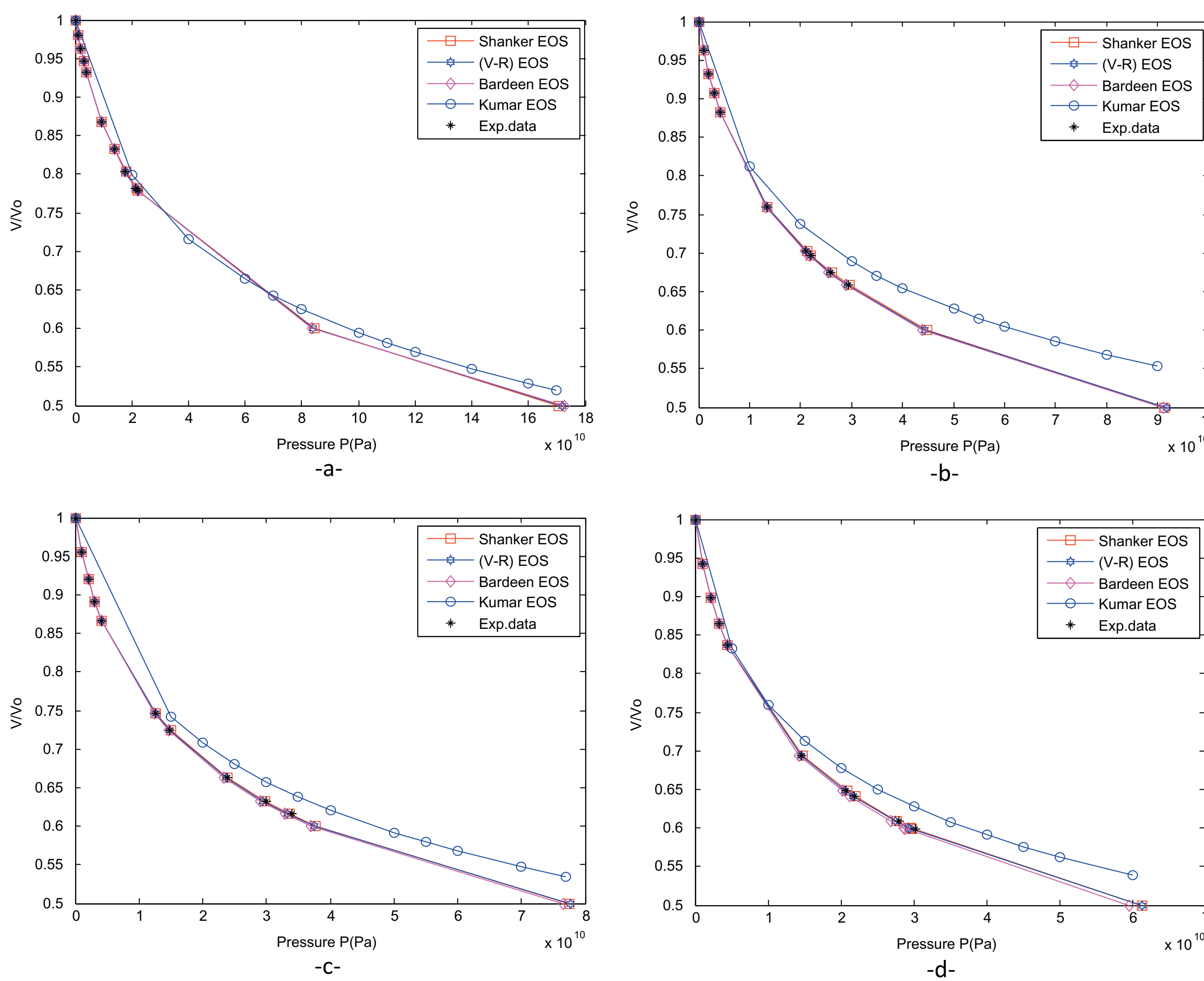

Figure 1 Comparison between the calculated isothermal compression curve at T = 300 K using four EOS with experimental data: (a) NaF (b) NaCl (c) NaBr (d) NaI.

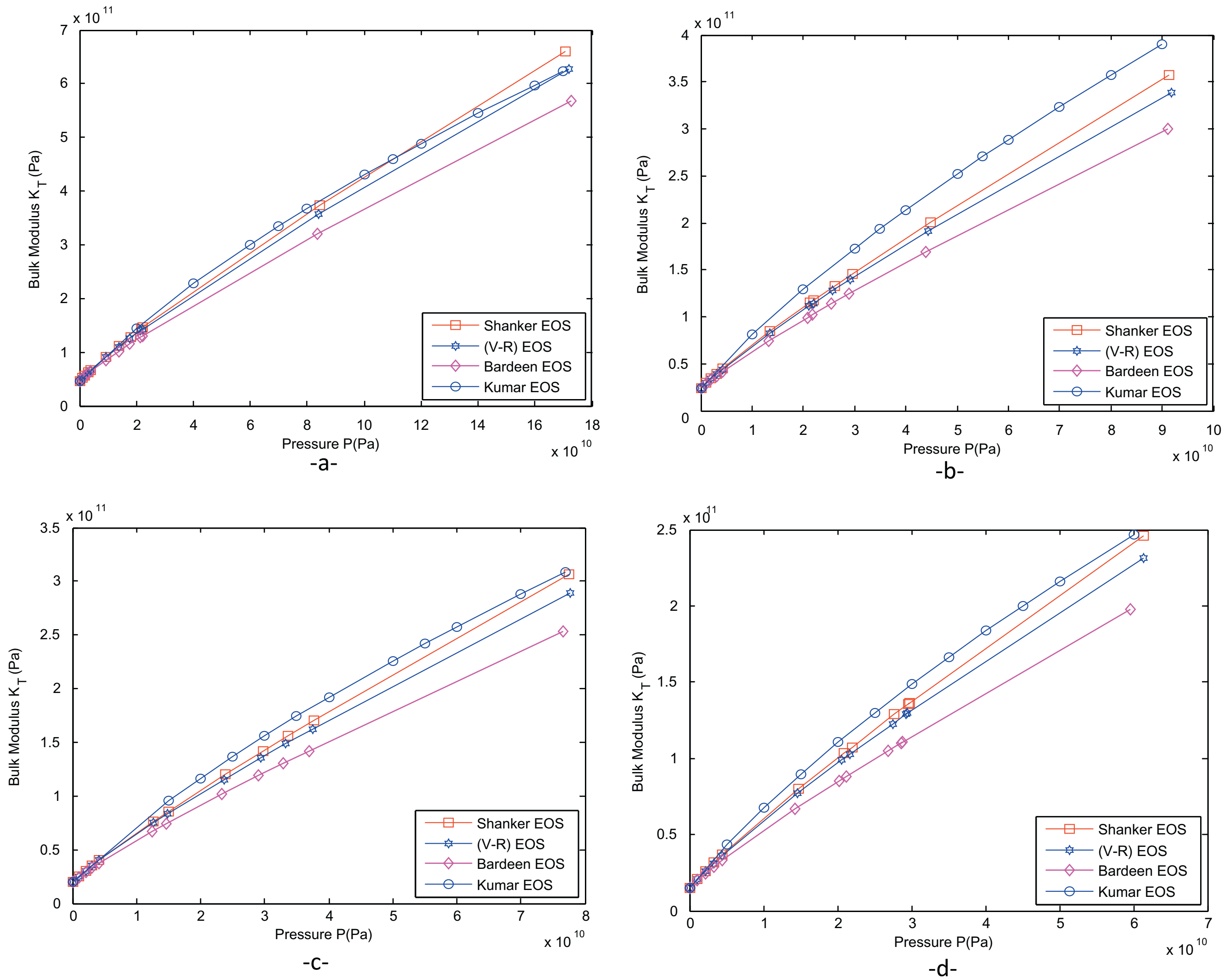

Figure 2 Isothermal bulk modulus versus pressure at $T = 300$ K using four isothermal EOS: (a) NaF (b) NaCl (c) NaBr (d) NaI.

2.3. Inverted Type EOS

There have been various attempts to propose inverted type EOS (non-isothermal) as reviewed by Freund and Ingalls (Freund and Ingalls, 1989). These EOS are based on different physical properties such as Kumari and Dass (Kumari and Dass, 1990), Kumar (Kumar, 1995), Bose-Roy and Bose-Roy, (Roy et al., 1999) and (Bose Roy and Bose Roy, 2004). However, the following EOS have been found to be the best way to describe the compression of solids at high pressure and temperature.

2.3.1. Kumar General EOS

Kumar (Kumar, 1995) and (Kumar, 1996) have obtained an inverted type EOS (non-isothermal) containing a term of temperature and in consequence valid for room temperature up to melting temperature, and at the pressure varying from atmospheric pressure up to the structural transition pressure.

Kumar General EOS is given below:

$$\frac{v}{v_0} = 1 - \frac{1}{A} ln\left[1 + \frac{A}{K_0}\{P - \alpha_0 K_0 (T - T_0)\}\right] \tag{14}$$

Or

$$P = \frac{K_0}{A}\left[expA\left(1 - \frac{v}{v_0}\right) - 1\right] + \alpha_0 K_0 (T - T_0) \tag{15}$$

where $A = (\delta_T + 1)$, δ_T is the Anderson–Gruneisen parameter, α_0 the coefficient of volume thermal expansion at room temperature (T_o) and δ_T is given below (Singh and Kumar,2004):

$$\delta_T = \delta_{T_0}\left(\frac{T}{T_0}\right)^s \cong K'_0 \tag{16}$$

δ_{T_0} is the value of Anderson–Gruneisen parameter at T_o and s is a dimensionless thermoelastic parameter whose value is about (1.4–1.5), as given by (Anderson et al., 1992), (Anderson and Isaak, 1993) for some alkali halides (from room temperature to melting temperature). In the present study we take $s = 1.5$.

2.3.1.1. Special Case. By assuming the temperature $T = T_o = 300$ K, Eq. (14) is reduced to the following form:

$$\frac{v}{v_0} = 1 - \frac{1}{A} ln\left[1 + \frac{A}{K_0} P\right] \tag{17}$$

or

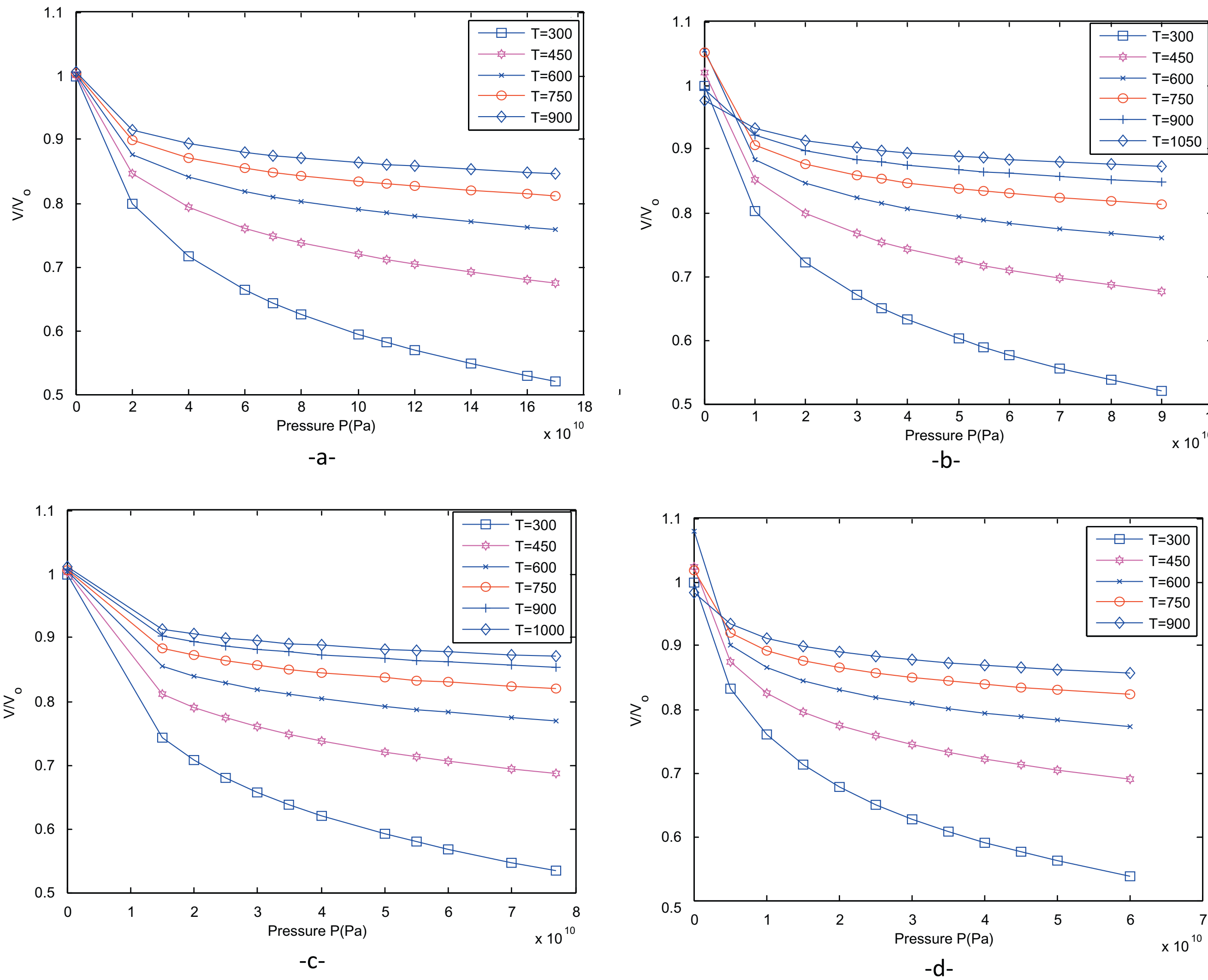

Figure 3 Non-isothermal curve at different temperatures using Kumar EOS: (a) NaF (b) NaCl (c) NaBr (d) NaI.

$$P = \frac{K_0}{A}\left[\exp A\left(1 - \frac{v}{v_0}\right) - 1\right] \tag{18}$$

Eq. (18) is the relation of $(\frac{v}{v_0})$ and (P) at constant temperature and therefore is called the isothermal equation of state.

The inverted type (non-isothermal) bulk modulus derived from Kumar General EOS Eq. (14) and from Eq. (4) is mentioned below:

$$K_T = K_0\left[1 - \frac{1}{A}\ln\left\{1 + \frac{AP}{K_0} - A\alpha_0(T - T_0)\right\}\left\{1 + \frac{AP}{K_0} - A\alpha_0(T - T_0)\right\}\right] \tag{19}$$

The isothermal bulk modulus derived from special Kumar General EOS Eq. (18) is given below:

$$K_T = K_0\left[\frac{v}{v_0} exp\left\{A\left(1 - \frac{v}{v_0}\right)\right\}\right] \tag{20}$$

3. Results and discussion

3.1. Isothermal Compression

The pressures have been calculated at different relative isothermal compression volumes ranging from 1 to 0.5 at $T = 300$ K for solid alkali halides (NaF, NaCl, NaBr and NaI) using (V–R) EOS, Shanker EOS, Bardeen EOS and Kumar isothermal EOS, Eqs. (12,6,9,18) respectively. The input parameters are listed in Table 1, where the values of K_0 and K'_0 are taken form (Roberts and Smith, 1970), α_0 is obtained from (Dhoble and Verma,1986) and δ_{T_0} from (Shanker and Singh, 1981). The results are shown in Fig. 1 and compared with experimental data obtained from (Sorensen, 1983).

From this figure one can see that the relative compression volume decreases continually with the increase in pressure. It is found that the results obtained from (V–R) EOS, Shanker EOS and Bardeen EOS are similar to each other and coincide with experimental data for four alkali halides. Although, the approach of the three equations is different, it indicates the validity of these models at low and high pressures. One can see from this figure that the values of applied high pressure for NaCl, NaBr, NaF and NaI at the compressibility (0.5) are equal to (90, 78, 170 and 60) GPa respectively. This is due to the pressure dependence on the bulk modulus (K_o) which has a lower value for NaI and a higher value for NaF. However, Kumar isothermal EOS results for four alkali halide solids at the compression range (1–0.75) are quit coincident with three EOS and experimental data. But at a range

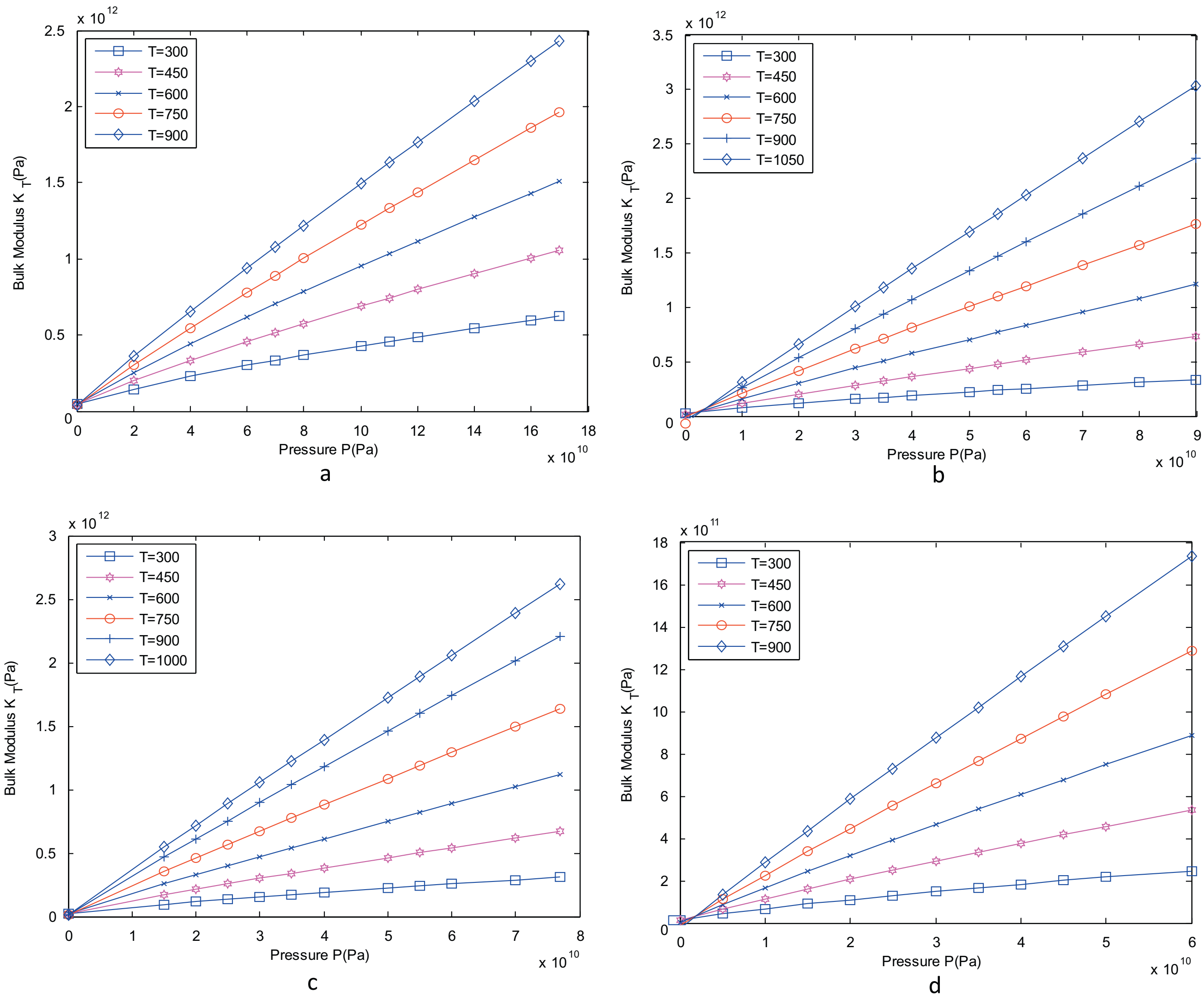

Figure 4 Non-isothermal bulk modulus versus pressure at different temperatures using Kumar EOS: (a) NaF (b) NaCl (c) NaBr (d) NaI.

(0.75–0.5), the results deviated from the other results. This indicates that Kumar EOS is not based on the interionic potential.

3.2. Isothermal bulk modulus

The isothermal bulk modulus (K_T) has been calculated at different relative compression volumes from 1 to 0.5 for four alkali halides using Eqs. (7,10,13,20). The input parameter values used are listed in Table 1.

Fig. 2 shows the isothermal bulk modulus (K_T) versus pressure (P) for (V–R) EOS, Shanker EOS, Bardeen EOS and Kumar isothermal EOS at $T = 300$ k. This figure exhibits that the isothermal bulk modulus (K_T) increases continuously with increase in pressure. In Fig. 2 one can see that, at low pressure the equations mentioned above coincide with each other. At high pressure, Fig. 2a shows that all equations diverge from each other. But in Fig. 2b and d, Shanker EOS and Kumar EOS coincide with each other, Fig. 2a shows that (V–R) EOS, Shanker EOS and Kumar EOS are converge to each other but Bardeen EOS diverge from them. Fig. 2b,c and d, show that at the pressure range (1–3GPa), the (V–R) EOS, Shanker EOS and Kumar EOS converge with each other, while Bardeen EOS diverge from those equations. At pressure range above 3GPa we shows four equations diverge to each other's.

3.3. Non-Isothermal Compression

The pressure has been calculated at different relative non-isothermal compression volume ranges (1–0.5) at different temperatures from $T = 300$ to temperature close to the melting temperature for solid alkali halides (NaF, NaCl, NaBr and NaI) using the Kumar General EOS Eq. (14). The input parameters are listed in Table 1. The relationships between compression and pressure (P) at different temperatures are plotted in Fig. 3. It has been seen from this figure that the compression (V/V_o) decreases with increasing pressure at a given temperature. However, the compression curve for all alkali halides increases as the temperature increases. This can be attributed to the volume expansion.

3.4. Non-Isothermal bulk modulus

The non-isothermal bulk modulus (K_T) has been worked out at different relative compression volumes (1–0.5) at different temperatures from $T = 300$ K to temperature close to the melting temperature for alkali halides (NaCl, NaBr, NaF and NaI) using the Kumar General EOS (Eq. (19)). The input parameters values used are listed in Table 1. The relationships between bulk modulus (K_T) and pressure (P) at different temperatures are plotted in Fig. 4.

In Fig. 4, it is clear that the bulk modulus (K_T) increases with pressure dramatically at a given temperature. (K_T) increases with (T) at a given pressure. When increasing the temperature the volume of solid increases and hence increases the bulk modulus. This increase is due to a coefficient of Anderson Gruneisen parameter, that contains the formula $(T/T_o)^s$ where its value increases with increasing the temperature.

4. Conclusions

In the present paper, the non-inverted (isothermal) type equations of state (EOS) which are based on interionic potential such as Vinet–Rydberg EOS, Shanker EOS, Bardeen EOS as well as Kumar isothermal EOS are used to study the variation of relative compression volumes in range (1–0.5) and the isothermal bulk modulus with high pressure at temperature T = 300 K for four alkali halides (NaF, NaCl, NaBr and NaI).

In this work, we have found that the relative compression volume obtained from the four EOS give a good agreement with experimental data up to 15 GPa. But beyond this point, the compression results stay in coincidence for the Vinet–Rydberg EOS, Shanker EOS and Bardeen EOS, while the results obtained from the Kumar isotherm EOS deviated from others EOS and from experimental data. Moreover, at the isothermal compression value 0.5, the calculated pressures for NaF, NaCl, NaBr and NaI were found to be 17, 90, 78 and 60 GPa respectively. Moreover, at the isothermal compression value 0.5, the calculated pressures for NaF, NaCl, NaBr and NaI were found to be 17, 90, 78 and 60 GPa respectively.

The results of isothermal bulk modulus for four EOS were found to be superimposed on each other at pressure from (0–1GPa). But beyond this value, the results of Vinet–Rydberg EOS and Shanker EOS are rather in good convergence. But the results of Bardeen EOS and Kumar EOS do diverge largely to other results.

However, the result of non-isothermal volume compression by using Kumar General EOS had shown that the compression curve for NaCl, NaBr, NaF and NaI increases as the temperature increases. This behavior also applied to the non-isothermal bulk modulus.

References

Anderson, O.L., 1995. Equations of State of Solids for Geophysics and Ceramic Science. Oxford University Press, New York.

Anderson, O.L., Isaak, D.G., 1993. The dependence of the Anderson Grüneisen parameter δ_T upon compression at extreme conditions. J. Phys. and Chem. Solids 54, 221–227.

Anderson, O.L., Oda, H., Isaak, D.G., 1992. A model for the computation of thermal expansivity at high compression and high temperature: MgO as an example. Geophys. Res. Lett. 19, 1987–1990.

Bardeen, J., 1938. Compressibilities of the alkali metals. J. Chem. Phys. 6, 372–377.

Birch, F., 1952. Elasticity and constitution of the earth interior. J. Geophys. Res. 57, 227–286.

Born, M., Huang, K., 1954. Dynamical Theory of Crystal Lattices. Oxford University Press, Oxford.

Bose Roy, S., Bose Roy, P., 1999. An equation of state applied to solid up to 1 TPa. J. Phys.: Condens. Matter 11, 10375.

Bose Roy, S., Bose Roy, P., 2004. An isothermal equation of state for solids. Physica B: Phys. Condens. Matter 350 (4), 375–388.

Butler, R., Anderson, D.L., 1978. Equation of state fits to the lower mantle and outer core. Phys. Earth Planet. Inter. 17, 147–162.

Dhoble, A., Verma, M.P., 1986. On the temperature variation of the Anderson–Grüneisen parameters of NaCl. Phys. Status. Solidi B 136, 497–504.

Digpratap, S., Rakesh, K., Arunesh, K., 2007. Analysis of temperature dependence of thermal pressure of solids. Indian J. Pure Appl. Phys. 45, 654–657.

Freund, J., Ingalls, R., 1989. Inverted isothermal equations of state and determination of B_0, B'_0 and B''_0. J. Phys. Chem. Solids 50 (3), 263–268.

Hama, J., Suito, K., 1996. The search for a universal equation of state correct up to very high pressures. J. Phys. Condens. Matter 8, 67–81.

Kumar, M., 1995. High pressure equation of state for solids. Physica B 212, 391–394.

Kumar, M., 1996. Application of high pressure equation of state for different classes of solid. Phys. B: Condens. Matter 217, 143–148.

Kumari, M., Dass, N., 1990. An equation of state applied to 50 solids. J. Phys. Condens. Matter 39, 3219, 2 7891.

Kushwah, S.S., Bhardwaj, N.K., 2009. Analysis based on equation of state for sodium halides. J. Phys. Chem. Solids 70, 700–702.

Kushwah, S.S., Shrivastava, H.C., Singh, K.S., 2007. Study of pressure–volume relationships and higher derivatives of bulk modulus based on generalized equations of state. Physica B 388, 20–25.

Poirier, J.P., Tarantola, A., 1998. A logarithmic equation of state. Phys. Earth Planet. Inter. 109, 1–8.

Roberts, R.W., Smith, C.S., 1970. The Anderson parameter and temperature dependence of bulk modulus for alkali halide crystals. J. Phys. Chem. 28, 1941, Sol., 31: 619, m. Sol.

Rydberg, R., 1932. Graphische darstellung einiger band spectroskopisher ergebriss. J. Zeitschrift fur Phys. 73, 376–385.

Shanker, J., Singh, K., 1981. Analysis of the crystal binding and the Gruneisen and Erson parameters in alkali-halides. J. Inorg. Nucl. Chem. 43 (7), 1445–1449.

Shanker, J., Kushwah, S.S., Kumar, P., 1997. Equation of state and pressure derivatives of bulk modulus for NaCl crystal. Physica B 239, 337–344.

Shanker, J., Kushwah, S.S., Sharma, M.P., 1999. On the universality of phenomenological isothermal equations of state for solids. Condens. Matter Physica B 271, 158–164.

Sharma, Uma., D., Joshi, H., Kumar, M., 2010. Effect of pressure and temperature on C60 fullerite. Indian J. Pure Appl. Phys. 48, 663–667.

Singh, P.P., Kumar, M., 2004. Temperature dependence of bulk modulus and second-order elastic constants. Physica B 344, 41–51.

Singh, R.K., Mitra, S.S., Rao, C.N., 1991. Temperature variations of the elastic constants of CaF_2 and SrF_2 crystals. Phys. Rev. B 44, 838.

Sorensen, Y.S., 1983. Phase transitions and equations of state for the sodium halides: NaF, NaCl, NaBr, and NaI. J. Geophysical Res. 88, 3543.

Sun, J.X., 2007. Equation of state and thermodynamic functions for the fcc soft-core multiple-Yukawa solid and application to fullerenes with compressible molecular radius. Phys. Rev. B 75, 035424.

Sushil, K., Arunesh, K., Singh, P.K., Sharma, B.S., 2004. Analysis of finite-strain equations of state for solids under high pressures. Physica B 352, 134–146.

Tosi, M.P., 1964. Cohesion of solids in the Born model. Solid State Phys. Adv. Res. Appl. 16, 1–120.

Vinet, P., Ferrante, J., Smith, J.R., Rose, J., 1986. A universal equation of state for solids. J. Phys. C 19, L467–L473.

Vinet, P., Rose, J.H., Ferrante, J., Smith, J.R., 1989. Universal features of the equation of state of solids. J. Phys. Condens Matter 1, 1941.