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Isothermal compression and thermal expansion of rhenium

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Abstract . A simple theoretical method based on the theory of equation of state is proposed to investigate the isothermal compression of rhenium upto V/V_0 = 0 734 Thermal expansion is reported from room temperature upto the melting temperature (T_m = 3453K) by varying the pressures from 0 to 200 GPa. The results are compared with the available experimental and theoretical data The good agreement obtained with the results based on the first principle calculations, support the validity of the present work

Keywords Isothermal compression, thermal expansion, rhenium

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Rhenium Re (Z = 75), widely spread throughout the earth's crust, has attracted the attention of theoretical [1] as well as experimental [2] workers. Re, a transition metal element crystallizes in hexagonal closed packed structure and is found to be stable [2] with the same structure upto its melting temperature (T_m = 3453 K) and no phase transition occurs upto the pressure 216 GPa. It has been used as a gasket material in high pressure diamond-anvil-cell experiment [3,4]. Because of its higher yield strength, it is expected to avoid "punch through" at the corners of the diamond until high pressurs are reached. An experimental analysis of Re has been performed by Vohra *et al* [2] to calibrate the ruby fluorescence method for pressure determination using X-ray diffraction method. Vohra *et al* used the isothermal equation of state (EOS) derived from shock wave data. Sikka and Kumar [1] have performed a critical study of the experimental results reported by Vohra *et al*. These authors [1] have used a first principle computation based on a linear muffin-tin orbital electron-band theory. It has been found that their calculated isotherm departs significantly from that derived from shock wave data [2]. However, the isotherm has been found to agree with the other isothermal EOS *viz*. Birch Murnaghan (BM) and Universal EOS. The disagreement between calculated and shock wave data has been discussed by Sikka and Kumar [1]. Moreover, the theoretical method [1] seems to be difficult and is limited to a particular temperature *viz*. isothermal condition. The method does not include the effect of higher temperatures, as generally occur in geophysical problems. Thus, it is legitimate and may be useful to point out some simple method which includes the effect of temperature also, which is the purpose of present work.

A simple theory of the behaviour of matter under extreme conditions has been reported by Kumar [5-7]. It has been found that the theory thus proposed, gives a better agreement [5-7] with the experimental data as compared with the Murnaghan, (BM) and Universal EOS. Due to the simplicity and applicability the theory is being frequently used in the literature [8-10]. The analysis of the theory is available elsewhere [7] and the mathematical form reads as follows [11, 12]

$$V \quad \cdot \quad {}^{1}\cdot \ln\left| 1+\frac{AP}{B_0} - A\alpha_0(T-T_0)\right|, \qquad (1)$$

where V/V_0 is the relative change in volume, P the pressure, T temperature, α the coefficient of volume thermal expansion, B the bulk modulus, O refers to their value at initial conditions *viz* at room temperature and atmospheric pressure. $A = (B_0' + 1)$, B_0' is the first order derivative of B with P. At reference temperature ($T = T_0$), eq. (1) is used to compute the values of V/V_0 at different P. The results thus obtained are reported in

Figure 1. In Table 1, I have quoted the numerical values of P corresponding to the $V/V_0 = 0.734$ which has been taken as a base point for comparison by earlier workers [12]. The results obtained in the present work are found in a good agreement

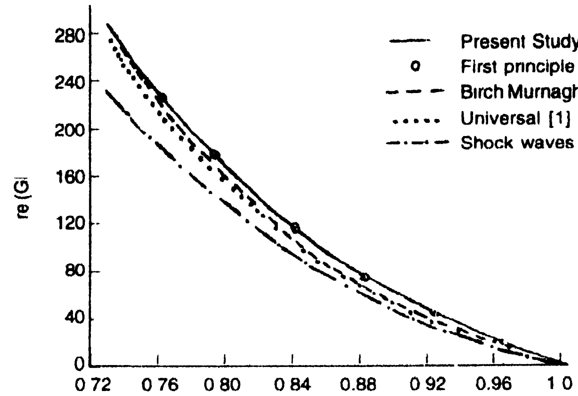

Figure 1. Isotherms obtained by different methods

with the results based on first principle calculations [1] and are far better than the BM and Universal EOS (Table 1). The shock isotherm is found to deviate largely. The possible reasons for such a deviation have been discussed by Sikka and Kumar [1].

Table 1. Comparison of pressure P (in GPa) obtained from different methods [1, 2] at the compression point ($V/V_0 = 0.734$), using $B_0 = 372$ GPa, and $B'_0 = 5.41$

	Method	P
1.	Shock isotherm	216
2	Birch-Murnaghan (BM) EOS	266
3	Universal EOS	257
4.	First principle calculation	264
5.	Present work	261

Vohra *et al* [2] used BMEOS for their analysis of shock wave data. It has also been concluded in the Jeanloz's papers [13, 14] that the third order BMEOS is the most successful among the other five polynomial forms in representing the shock wave data. Thus, it is difficult to doubt on BMEOS. Actually, the value of $B_0' = 4.05$ obtained by Vohra *et al* [2] seems to be doubtful. Not only Vohra *et al* [2] but some other authors [15,16] have also taken $B_0' = 4$ in high pressure measurements, which is a crude approximation. The value of B_0' reported by Vohra *et al* is very close to 4. Here, it should be mentioned that $B_0' = 4$ is not acceptable in BMEOS because it disturbs the mathematical form of the EOS. This may be understood by looking into the mathematical form of the EOS which reads as [2, 7]

$$P = 3B_0 f(1+2f)^{5/2}\left[1+\frac{3}{2}(B_0'-4)f\right], \qquad (2)$$

where $f = \frac{1}{2}\left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]$

Now, if I put $B_0' = 4$ in eq. (2), it becomes

$$P = 3B_0 f(1+2f)^{5/2} \qquad (3)$$

Eq. (3) which is a special case of BMEOS, may be valid only for low pressure ranges (about 10 GPa). On the other hand, eq. (2) [in which $B_0' \neq 4$] is found to work in high pressure ranges [17-20]. Vohra *et al* [2] used eq. (2) and found $B_0' \simeq 4$. Thus, their results are equivalent to eq. (3). Walzer [21] studied Hugoniot curve using a semitheoretic approach and reported $B_0' = 5.388$. Walzer's value of B_0' is in agreement with the ultrasonic measured value of $B_0' = 5.41$ as quoted by Steinberg [22]. Sikka and Kumar [1] have also taken $B_0' = 5.41$ and $B_0 = 372$ GPa [2] for their studies. In view of the above, the author has accepted $B_0 = 372$ GPa and $B_0' = 5.41$ as model parameter.

Here, it should be mentioned that the model considered in the present paper is consistent with the equilibrium condition [5-7]. Eq. (1) is also used to study the temperature dependence of V/V_0 at different pressures using $\alpha_0 = 18.6 \times 10^{-6}$ K^{-1} as given by Lide [23]. The results thus obtained are reported in Figure 2. The values of V/V_0 are found to increase by increasing T. However, this increase becomes less as pressure is increased. When the temperature and pressure are very high, the variation of V/V_0 is very small. It seems that the effect of temperature is being cancelled by the effect of pressure. These results are reported in the absence of experimental data, may be helpful for planning the new experiments in the field of high pressure and high temperature. Such results are of urgent need for the geophysical analysis of rhenium [23].

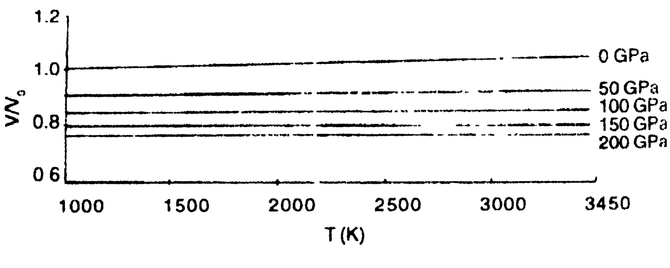

Figure 2. Thermal expansion at different pressures using eq (1)

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