

## Analysis of thermal expansivity of iron (Fe) metal at ultra high temperature and pressure

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**Abstract.** In the present investigation we have explained the thermal and compression properties of HCP iron (Fe) at high pressure with variable temperature (isobars) and at high temperature with variable pressure (isotherm). The usual Tait equation of state is modified by incorporating the effect of thermal pressure. The calculated values of pressure for different isotherms and isochores and thermal expansivity ( $\alpha$ ) as a function of both temperature and pressure have been compared with those values obtained by Isaak *et al* and Wasserman *et al*.

**Keywords.** Thermal expansion; expansivity; hexagonal close packed iron.

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### 1. Introduction

It is a well-known fact that the hexagonal close packed (HCP) iron is a major core component of the Earth's deep interior. Therefore, the study of the thermal properties of iron at extreme pressures and temperatures of the Earth's core are very important for understanding the dynamics of the core [1,2]. Our motive is to determine the volume coefficient of thermal expansion ( $\alpha$ ) for HCP iron over a wide range of temperature and pressure. During the past years various theoretical potential models [3–6] have been employed to study the thermal properties of iron at high temperatures and pressures. The band structure calculation shows a good description of the static equation-of-state and the low temperature phase diagram of iron [4]. The study of high temperature properties, however, is not reasonable with linearized augmented plane wave method as the simplified models of the electronic structure are unlikely to be successful for predicting the high temperature properties of transition metals due to the complicated many-body nature of the interactions. Wasserman *et al* [3] have recently studied the thermal properties of iron at high pressures and temperatures within the framework of shell model [7,8], which is well applicable above the Debye temperature where vibrational states are essentially

fully populated. The model used by these workers is too good to predict the thermal properties of iron at high temperatures and pressures through heavy computational work that is involved in their calculation.

In the present paper the authors provide a simple and straightforward method, based on thermodynamic variables, to determine the thermodynamic properties of transition metals, for example, HCP iron. We have made use of Tait's equation-of-state commonly known as usual Tait equation-of-state (UTE) [9,10] in its modified form which includes the effect of thermal pressure ( $P_{th}$ ) at high temperatures. The anharmonic (non-linear) term arising due to the thermal excitation of electrons [11,12] at high temperature has been taken into account in the expression of thermal pressure ( $P_{th}$ ) [13]. The results calculated in the present study are compared with those obtained by Wasserman *et al* [3] and Isaak *et al* [13].

## 2. Method of determination of $\alpha$ for HCP iron

The original usual Tait equation-of-state (UTE) for relative compression with pressure can be written as [9,10]

$$\frac{V}{V_0} = 1 - \frac{1}{K'_0 + 1} \ln \left[ 1 + \frac{K'_0 + 1}{K_0} (P) \right]. \quad (1)$$

Due to the internal thermal pressure  $P_{th}$  developed at the walls of the unit cell of the crystal at high temperature, eq. (1) can be modified in the following form:

$$\frac{V}{V_0} = 1 - \frac{1}{K'_0 + 1} \ln \left[ 1 + \frac{K'_0 + 1}{K_0} (P - P_{th}) \right], \quad (2)$$

where  $P_{th}$  is the thermal pressure resulting due to high temperature, which can be defined as

$$P_{th}(V, T) = \int_{T_0}^T \alpha K_T dT. \quad (3)$$

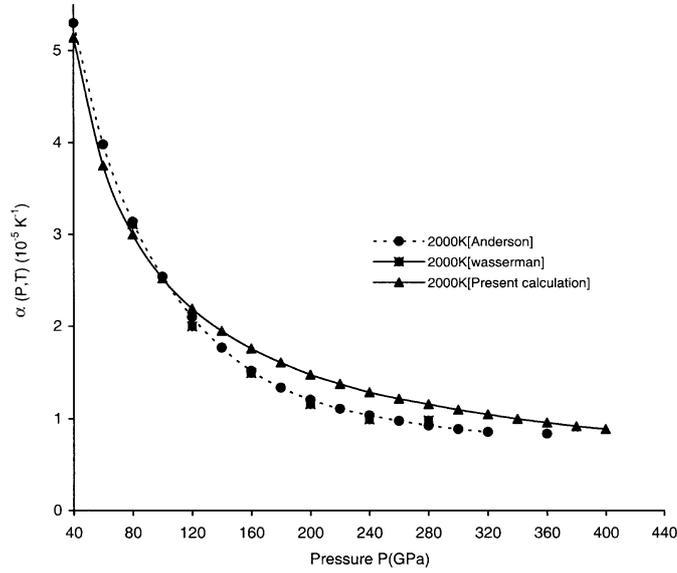
On differentiating eq. (3) we get

$$\left( \frac{\partial P_{th}}{\partial T} \right)_V = \alpha K_T. \quad (4)$$

The product of  $\alpha K_T$  in the RHS of eq. (4) is generally assumed to be nearly constant for non-metals in high temperature equation-of-state. In this approximation  $P_{th}$  is proportional to  $\Delta T = T - T_0$  with  $\alpha K_T$  being the proportionality constant. However, for metals, the thermal pressure  $P_{th}$  cannot be assumed as a linear function of temperature due to the thermal excitation of electrons [11,12] which includes a higher order term. In other words,  $\alpha K_T$  (not  $P_{th}$ ) is the linear function of  $T$  [3,13,14] and the integration of eq. (4) gives [13]

$$P_{th}(T) = a(\Delta T) + \frac{1}{2}b(\Delta T)^2 \quad (5)$$

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**Figure 1.**  $\alpha(P, T)$  vs. pressure at temperature  $T = 2000$  K for Fe.

or

$$P_{\text{th}}(T) = a(T - T_0) + \frac{1}{2}b(T - T_0)^2, \quad (6)$$

where  $a$  and  $b$  represent  $(\alpha K_T)_{300 \text{ K}}$  and  $(\partial \alpha K_T / \partial T)_V$ , respectively. The value of  $\alpha$  and  $K_T$  at 300 K for HCP iron has been taken from ref. [13]. However, the value of the anharmonic coefficient  $b$  is calculated from the slope of the graph plotted between the products of  $\alpha K_T$  vs. temperature which is found to be  $0.774 \text{ Kpa K}^{-2}$  very close to the value given in refs [13,14].

The values of  $\alpha(P, T)$  for HCP iron (Fe) have been calculated by making use of the equation-of-state (2). On substituting the values of  $V/V_0$  (eq. (2)) in the following equation [16]

$$\alpha(P)_T = \alpha_0 \frac{V_0}{V} \left[ \exp(K'_0 + 1) \left( \frac{V}{V_0} - 1 \right) \right]. \quad (7)$$

The resulting values of  $\alpha(P)$  along selected isotherms are illustrated in figures 1–3. The thermal expansion coefficient  $\alpha(T)_P$  for different isobars has been calculated from the equation as described above. The calculated values of  $\alpha(T)$  are compared with those obtained by Isaak *et al* [13] as illustrated in figure 4.

### 3. Results and discussion

It may be noted from figures 1–3 that our results deviate systematically from Isaak and Wasserman theories only in higher-pressure range especially at 2000 K. The

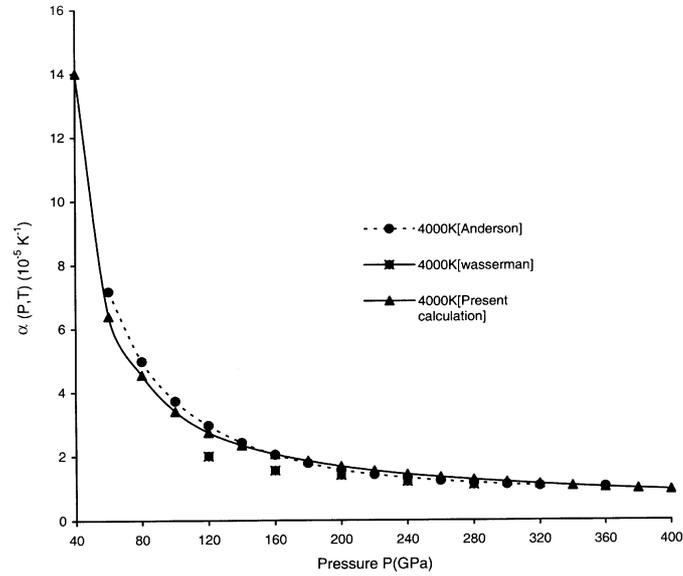


Figure 2.  $\alpha(P, T)$  vs. pressure at temperature  $T = 4000$  K for Fe.

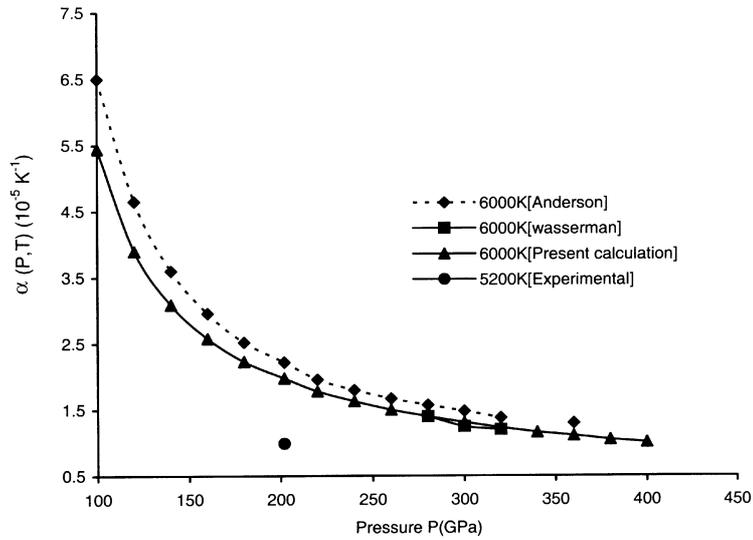


Figure 3.  $\alpha(P, T)$  vs. pressure at temperature  $T = 6000$  K for Fe.

deviation in this region may be ascribed to the fact that the value of the parameter  $a = 12.84 \times 10^{-3} \text{ GPa K}^{-1}$  used in eq. (6) is higher than the value  $6.9 \times 10^{-3} \text{ GPa K}^{-1}$  as reported by Uchida *et al* [17] for HCP iron based on analysis of new experimental data. Wasserman *et al* have considered this value at about  $11.5 \times 10^{-3} \text{ GPa K}^{-1}$  at 2000 K. However, the anharmonic coefficient  $b$  and the temperature

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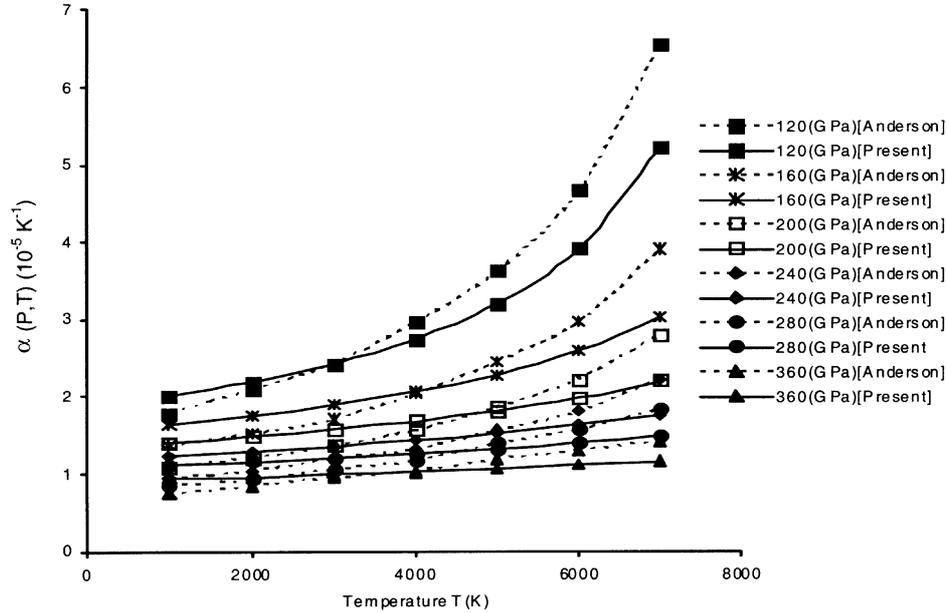


Figure 4.  $\alpha_T$  vs. temperature at different isobars for Fe.

derivative of the product of  $\alpha$  and  $K_T$  at 300 K as considered in the non-linear term (eq. (6)) has been taken as the same value, i.e.  $0.78 \text{ Kpa K}^{-2}$  as used by Stixrude *et al* [15].

Values of  $\alpha(T)$  for different isobars of HCP iron (Fe) have been calculated in the present study from the same thermal pressure equation in which the values of  $V/V_0$  is now read as thermal expansion instead of compression. The values of thermal expansion are determined from eq. (2) for different isobars at different high temperatures. It is also clear from figure 4 that the value of thermal expansion coefficient found in our calculation is more close to the shock Hugoniot value [18] as compared to that of Isaak *et al* [13]. This value  $0.91 \pm 0.20 \times 10^{-5} \text{ K}^{-1}$  was reported at  $202 \pm 3 \text{ GPa}$  and  $5200 \pm 500 \text{ K}$ . Our results calculated from the present thermal pressure equation-of-state (7) is about  $1.70 \times 10^{-5} \text{ K}^{-1}$  where this value determined by Isaak *et al* is about  $1.80 \times 10^{-5} \text{ K}^{-1}$  at the same pressure and temperature conditions.

On the basis of the overall description it may be concluded that our results for  $\alpha(P, T)$  calculated from the modified usual Tait equation-of-state (UTE) are found in remarkable agreement between the two theories [3,13] throughout a wide range in both  $P$  and  $T$ . It is found in the present work that the value of  $\alpha$  at 202 GPa and 5200 K is higher than the shock Hugoniot value  $0.91 \pm 0.2 \times 10^{-5} \text{ K}^{-1}$  [18].

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