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Optimum values of Second Grüneisen parameter (q) for Iron, Vanadium and Titanium

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الخلاصة

في هذا البحث تم صياغة نموذج امثلية عددية يستخدم القيم التجريبية لتأثير الضغط على الجزء الخالي من الارتداد، باستخدام علاقة مطورة بين درجة حرارة ديباي والحجم المعتمد على معامل كرونيشن γ , والمعامل الثانى لكرونيشن q ، اذ امكن استنتاج القيم المثلى لـ q لكل من الحديد، الفاناديوم والتيتانيوم .

ABSTRACT

In the present work a numerical model is constructed for the joint optimization of experimental data on recoilless fraction, using an improved relation between Debye temperature and the volume dependence of Grüneisen parameter γ, and the second Grüneisen parameter q. This model shows the optimum q values for Iron, Vanadium and Titanium.

1. INTRODUCTION

The thermodynamic properties of solids under pressure attracted extensive attention in the field of material science, engineering, geophysics, and so on (Xie et al, 1999). The Grüneisen parameter γ has been widely used to characterize and extrapolate the thermo physical properties of materials to high pressure and high temperature. The volume dependence of Grüneisen parameter on volume given, (Boehler, 1983), as

$$\gamma = \gamma_o \left(\frac{V_p}{V_o}\right)^q \qquad \ldots(1)$$

where:

subscript (o) implies values at reference condition (298K) q-2nd Grüneisen parameter.

Intensive theoretical research in the field of the pressure dependence of Grüneisen parameter in the recent years (Anderson, 1974 ; Anderson & Isaak, 2000; Al-Sheikh et al., 2005) has led to a somewhat better understanding of solids under pressure.

Available data on the variation of Grüneisen parameter with volume for vanadium and titanium are very rare while that for iron are limited and not in complete agreement with each other (Table-1).

McQueen et al. (1970) provided the Grüneisen parameter to more than 100 Gpa based on finite differences in thermal pressure between porous and non-porous Hugoniot data. They found q= 1 to be reasonable approximation to their scattered data. Jeanloz (1979) reconsidered the same porous Hugoniot data proposed q is equal to 1.62. Boehler et al., (1979) calculated γ for quartz from the adiabatic pressure derivative of

Temperature $(\frac{\partial T}{\partial p})_s$ by use of thermodynamic relationship

$$\gamma = \frac{B_s}{T}\left(\frac{\partial T}{\partial p}\right)_s \qquad \ldots(2)$$

Where B_s is the adiabatic bulk modulus. They found parameter γ decreases wIth pressure and value for $q = -(\frac{\partial \ln \gamma}{\partial \ln V})_T$ of 2.0.

Table -1- : Volume Dependence of γ and q

Material		γ_o	q	Reference
Iron ε-phase	15-100Gpa	2.2	1.0	McQueen et al., (1970)
	15-100Gpa	2.2	1.62	Jeanloz, (1979)
	0-240Gpa	1.7	0.7	Anderson, (1998)
	0-300Gpa	1.78	0.69	Dubrovinsky, (2000)
	200Gpa	1.9	1.0	Anderson, (1974)
Iron α-phase	0-10Gpa	1.66	0.6	Boehler &Ramakrishnan, (1980)
		1.69	0.8	Anderson &Isaak, (2000)
		1.66	0.6	
		1.66	**0.78**	**Present work**
Iron γ_i-phase	0-100Gpa	1.4	1.5	Anderson, (1974)
Quartiz		0.675	2.0	Boehler et al., (1979)
Al		2.14	1.0	Hänström & Lazor (2000)
In		2.42	1.8	Boehler & Ramakrishnam, (1980)
Pb		2.63	1.2	
Na		1.2	0.91	
K		1.19	1.7	
Bi		1.0	1.4	
Cu		2.01	1.3	
		1.96	1.0	Al-Sheikh et al., (2005)
Ti		1.232	1	Al-Sheikh & Al-Saydia, (2002)
			2	
			1.12	**Present work**
V		1.257	1	Al-Sheikh & Al-Saydia, (2002)
			2	
			1.01	**Present work**
NaCl		1.64	1.46	Dass&Kumari, (1984)
			1.10	
			1.40	

* $\gamma_i \Rightarrow$ indicate γ-phase for Iron $\gamma_o \Rightarrow$ indicate Grüneisenn parameter at reference pressure.

Boehler and Ramakrishnan (1980) measured γ as a function of pressure for various materials using the adiabatic decompression method and found γ_0 and q (Table-1). Dass and Kumari (1984) reported q=1.46, 1.10 and 1.4 for Nacl. Brown and McQueen (1986) found that for liquid iron $\gamma_0 = 1.59$. In their study, equation of state for gold, Anderson et al. (1989), suggested value of q is near (2.5-3), in order to ensure thermodynamic consistency.

Using semi-empirical consideration, Stacey (1995) found that the value of γ = 1.27-1.33 for closed - packed crystalline iron at the pressure range of the outer core. Based on the analysis of Stacey (1995), Anderson (1998) suggested the value of γ_0=1.7 and q = 0.7 for ε-iron. Dubrovinsky et al. (2000) determines the Grüneisen parameter for ε-iron on the basis of atom's mean square displacement from high pressure and temperature x-ray investigations.

Al-Sheikh and Al-Saydia, (2002) in their study variation of Dedye temperature with pressure, estimated q = 1 & 2 for both vanadium and titanium. Based on the theoretical analysis of effect of pressure on traction for Mossbauer source Fe57 in natural iron, Al-Sheikh and Al-Khero (2003) suggested $\gamma_0 = 1.661$ and q = 1 for iron. The present work construct a numerical model for the joint optimization of experimental data on the recoilles traction, pressure, Debye temperature, Grüneisen parameter (γ), and second Grüneisenn parameter (q).

2. Theory and Results:

In the Mie- Grüneisen theory the γ-parameter is defined (Boehler & Ramakrishnan, 1980) as

$$\gamma = \frac{\alpha_V . B_T}{C_V . P} = \frac{\alpha_V . B_S}{C_P . \rho} \qquad \ldots(3)$$

α_v- volume coefficient of thermal expansion
B_T, B_s- isothermal and adiabatic bulk moduli.
C_p, C_v - specific heat at constant pressure and constant volume
ρ - density

It is extremely difficult to measure precisely the pressure dependence of (α_v, B_T, C_v and C_p

The γ-parameter is calculated (Boehler et al., 1979) using the thermodynamic relation

$$\gamma = \frac{B_S}{T} \left(\frac{\partial T}{\partial P}\right)_S \qquad \ldots(4)$$

The pressure dependence of γ is very often expressed in the form of equation (1). γ decrease with pressure for all solids except when a substance undergoes a phase transition. The values of q depend some what on the source of the B_s data. Anderson (1974, 1979) lists value of q for various materials calculated from the thermodynamic relation ship

$$q=-\frac{1}{B_S\alpha_V}\left(\frac{\partial B_S}{\partial T}\right)-B'_S+\gamma+1 \qquad \text{...(5)}$$

In this work we couple the frequently used power law relationship of eq. (1) with Murnaghan equation of state (Angel, 2001).

$$\frac{V_P}{V}=\left(1+\frac{B'P}{B_{0S}}\right)^{-\frac{1}{B'}} \qquad \text{...(6)}$$

P- pressure in kbar an B_{0s}adiabatic bulk modulus

$B'=\frac{\partial B}{\partial P}$ - pressure derivative of bulk modulus.

If γ dependent on volume (eq.1), the relationship between. The Debye temperature and volume is given as (Dubrovinsky et al., 2000)

$$\ln\theta_P=\ln\theta_D+\frac{\gamma_o}{q}\left[1-\left(\frac{V_P}{V_o}\right)^q\right] \qquad \text{...(7)}$$

θ_D,θ_P-Debye temperature at atmospheric and P- pressure respectively .

In Debye approximation, f-fraction expressed as (Al-Sheikh & Al-Saydia, 2002).

$$f_P=\exp\left[-\frac{E_R}{K_B\theta_P}\left(\frac{3}{2}+\frac{\pi^2T^2}{\theta_P^2}\right)\right] \quad , \quad T<\theta_D \qquad \text{...(8.a)}$$

$$f_P=\exp\left[-\frac{6E_R}{K_B\theta_P^2}\right] \quad , \quad T>\theta_D \qquad \text{...(8.b)}$$

Where

E_R- recoilless energy

K_B-Boltzmann constant

T = 298 K

The result of optimum q-values, shown in Fig-1 and tabulated in (Table-1) for the present work are obtained by optimization of experimental data, for Fe (South well et al., 1968); V & Ti (Moyzis, 1968), on recoilles fraction (f-fraction) under pressure using Debye approximation. A numeric model constructed, combining equations 6,1,7 and 8 for the joint of experimental and theoretical calculations evaluated using data for B, B' and θ_D in Table -2.

Table -2

Bulk modulus (B_{os}), pressure derivative of Bulk modulus B' and Debye temperature for iron, vanadium and Titanium

Material	B K bar	B'	θ_D	Ref.
Fe	1627.2	5.9	453	Mao et al., 1967
V	1551	4.504	273	Alers, 1960
Ti	1074	1.353	385	Fisher & Renken, 1964

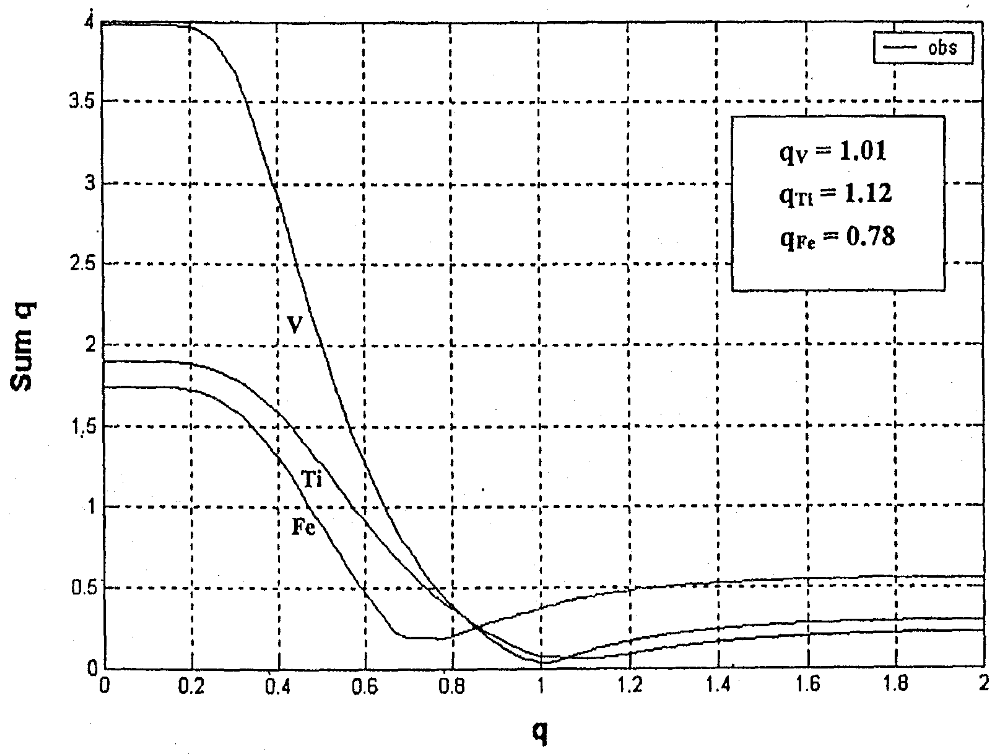

Fig. (1) : Optimum q values for Iron, Vanadium and Titanium

4.Discussion

Anderson and Isaak, 2000, combines the lindemann melting equation with the vient isothermal equation of state by means of the Grüneisen parameter γ a long the melting cure of α-iron, found q=0.6, 0.8 (Table-1) . In the present work the optimum q values 0.78, 1.01 and 1.12 for α-Fe, V and Ti indicate a good agreement with Anderson and Isaak, 2000.

Our numerical model couple the general form of Murnagphan, equation of state & Grüneisen parameter in the improved θ_D volume dependence

$$\ln\theta_D = \ln\theta_D + \frac{\gamma_o}{q}[1 - (\frac{V_P}{V_o})^q]$$

Besides the construction of optimization procedure for q values on evaluation f-fraction of equations 6.

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