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Pressure-volume Relationship for Platinum and Aluminium

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Abstract

Platinum and Aluminium are widely used as a pressure calibration standard. The present proposal which intends to compare the efficiency of the four equations under close examination reports the V/VO versus P values derived from the new modified forms of Murnaghan equation NMME1, NMME2, Birch equation (BE) and Freund-Ingalls (FIE) obtained for the best agreement with the experimental data of Mc Queen et.al.

Key Words: Equation of state, NMME1, NMME2, BE, FIE
PACS numbers: 64.30.-t; 64.10.+h; 62.20.-x

Introduction

The materials included in this study are Platinum and Aluminium and have been investigated up to extremely high pressures via the shock wave technique [1] and retain their phase over the respective pressure range investigated. Platinum is among the densest elements (ρ~20gm/cc). The metal does not exhibit any anomalies in the shock velocity-particle velocity relation up to pressures as high as 300GPa. The high pressure change their electronic states from normal metals below about 200 GPa to hot dense plasma state above 5 TPa with intermediate states of condensed liquid and cold plasma. A systematic pressure volume relationship through these states can be extremely useful for the measurement of pressure through the entire range. We have investigated these materials mainly for the purpose.

Theory and Calculations

Some physical properties of Platinum and Aluminium are listed below. The properties included are (i) the structure with lattice constants a and c (ii) the zero pressure density ρ_0 and (iii) the max. pressure P_{max} reached in the particular study and the original reference.

Material	a,c(A°)	ρ_0	P_{max}
Pt	F.C.C	21.42	58.6 [2]
	a=3.92		270 [1]
			430 [3]
			660 [4]
Al	F.C.C	2.78	50.5[2]
			100 [5]
	a=4.05		120 [5]
			150 [6]

The values of B_o, $B_o`$ and $B_o``$ as determined from the polynomial fit with the p-v data are listed below,

Pt: B_O (GPa) = 277.1; $B_O`$ = 4.438; $B_O``$ (GPa^{-1}) = 0.0352

Al: B_O (GPa) = 78.34; $B_O`$ = 3.147; $B_O``$ (GPa^{-1}) = 0.109

The values have been numerically determined from equations as,

$$B = -V\left(\frac{dP}{dV}\right) \quad (1)$$

$$B = -\frac{1+\sum_i ai\,(P)^i}{\sum_i iai\,(P)^{i-1}} \quad (2)$$

In the limit P=0, we get

$$B_O = -\frac{1}{a_1} \quad (3)$$

Successive differentiation of eqn. 1 with respect to P and then on taking the limit as P=0 yield

$$\frac{dB}{dP} = B_O` = -1 + \frac{2a_2}{{a_1}^2} \quad (4)$$

$$\frac{d^2B}{dP^2} = B_O`` = \frac{2a_2}{a_1} + \frac{6a_3}{{a_1}^2} - \frac{8{a_2}^2}{{a_1}^3} \quad (5)$$

and so on. The suffix o indicates value at zero pressure. It is observed that contrary to expectations $B_o``$ is positive in this case. However, numerical values of $B_o``$ evaluated at high pressures show that this derivative takes negative values for the entire pressure range starting from P=20 or 30 GPa that is

nearly the zero pressure. The positive values may therefore be due to small undulations caused by the numerical programme. The shock wave data published by McQueen et al [1] covers a pressure range for the normal metal phase of these materials. The p-v data tabulated by these authors were used to obtain the best fit parameters for the four equations under examination namely the NMME1 [7], NMME2 [7], FIE [8] and BE [9]. The two equations which have been designated as NMME1 and NMME2 indicate that they are new modified forms of Murnaghan equation. The Freund-Ingalls three parameter equation FIE [8] and the Birch equation BE [9] have also been used for comparing the derived equations [7] with these two equations which are known to be giving very good results in similar studies. The equations used for fitting the p-v data are explicitly given here for ready reference.

$$P = \left(3\frac{B_0}{2}\right)\{(\frac{V_0}{V})^{\frac{7}{3}} - (\frac{V_0}{V})^{\frac{5}{3}}\}\{1 + (\frac{3}{4})(B_0` - 4)[(\frac{V_0}{V})^{\frac{2}{3}} - 1]\} \quad (6)$$

(Birch equation)

$$\frac{V}{V_0} = \{1 - a\ln(1 + bP)\}^c \quad (7)$$

(Freund and Ingalls equation)

$$\frac{V}{V_0} = (1 + p)^{-\frac{1}{n}}[1 + (\frac{m}{6n})\{b(p + 1)^2 + 3(1 - 2b)(p + 1) + 3b - 6(1 - b)\ln(p + 1) - \frac{(3-2b)}{(p+1)}\}] \quad (8)$$

(New modified form of Murnaghan equation NMME2)

This equation easily goes into NMME1 for b=1

Results

The present study which intends to compare the efficiency of the four equations under close examination reports the V/V_O versus P values derived from the NMME1, NMME2, BE and FIE obtained for the best agreement with the experimental data of Mc Queen et.al. The shock wave data published by McQueen et.al covers a pressure range for the normal metal phase of these materials. These values are reported in (Tables 1&2).

Table 1. Pressure versus volume of Platinum

P (GPa)	Expt.	NMME1	NMME2	FIE
0	1	-	-	-
10	0.967	-	-	-
20	0.9395	-	-	-
30	0.9162	-	-	-
40	0.8955	-	-	-
50	0.8775	-	-	-
60	0.8609	-	-	-
70	0.8463	-	-	-
80	0.8328	-	-	-
90	0.8204	-	-	-
120	0.7878	0.7878	0.7878	0.7878
150	0.7612	0.7614	0.7616	0.7612
180	0.7389	0.739	0.7393	0.739
210	0.7193	0.7196	0.7199	0.7198
240	0.7023	0.7025	0.7028	0.7031
270	0.6874	0.6871	0.6875	0.6883

Table 2. Pressure versus volume of Aluminium

P(GPa)	Expt.	NMME1	NMME2	BE
0	1	1	1	1
10	0.8997	0.9001	0.9001	0.9013
20	0.8348	0.835	0.835	0.8358
30	0.7875	0.7875	0.7875	0.7877
40	0.7514	0.7505	0.7504	0.7501
50	0.7202	0.7203	0.7203	0.7196
60	0.695	0.6949	0.6949	0.6941
70	0.6731	0.6731	0.6731	0.6722
80	0.6541	0.6539	0.6539	0.6532
90	0.6362	0.6368	0.6368	0.6364
100	0.6205	0.6214	0.6214	0.6214
110	0.607	0.6073	0.6073	0.608
120	0.5953	0.5943	0.5943	0.5658

The graphs obtained by plotting these values against P together are shown in (Figures 1 & 2).

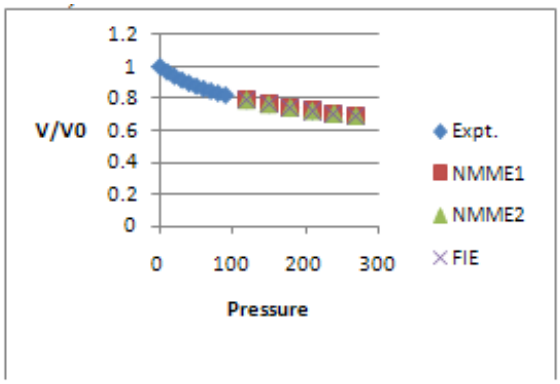

Figure 1. Pressure versus relative volume of Pt.

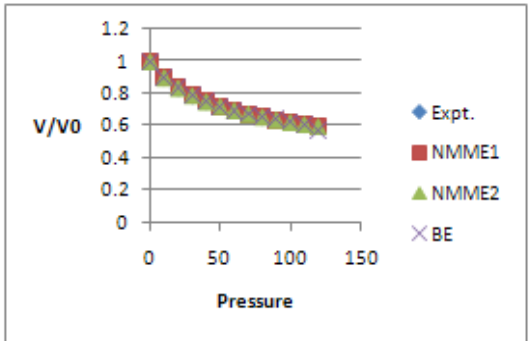

Figure 2. Pressure versus relative volume of Al.

The best fit values for B_O, $B_O`$, $B_O``$ and $B_O```$ are listed in (Tables-3&4).

Table 3. The zero pressure bulk modulus and its pressure derivatives for Pt

Bo	Bo`	Bo``	Bo```	Source
279.8	4.7	-	-	BE
279.53	4.57	$-7.018*10^{-4}$	-	NMME1
278.76	4.6	$-7.34*10^{-4}$	$2.5*10^{-5}$	NMME2
282.043	4.46	$-7.018*10^{-4}$	-	FIE
283.8	-	-	-	Ref.[10]
282.7	-	-	-	Ref.[11]

Table 4. The zero pressure bulk modulus and its pressure derivatives for Al

Bo	Bo`	Bo``	Bo```	Source
78.2	4	-	-	BE
77.3	3.804	$-1.759*10^{-3}$	-	NMME1
77.273	3.805	$-1.759*10^{-3}$	$-1.735*10^{-4}$	NMME2
79.4005	3.596	$-1.759*10^{-4}$	-	FIE
75.7	-	-	-	Ref.[5]
76.9	-	-	-	Ref.[12]
73.58	-	-	-	Ref.[9]
-	4.85	-	-	Ref.[13]

Conclusion

The numerical results clearly show that the p-v data, of the materials included in this study, upto moderately high pressures of the order of a few hundred GPa are explained very well with several equations of state. Equation NMME1 further shows that the modification in the simple two parameter Murnaghan equation is rather small. To have an exact estimate of the change that is produced by the NMME1 in the ME one has only to evaluate the term $\lambda_u = mp^3/6n(p+1)$ which adds to one and then multiplies the ME expression $(1+p)^{-1/n}$ to yield the volume ratio V/V_0. The values of λu at the highest pressures investigated have been calculated and listed below for the solids under examination.

Pt= -0.0054

Al= -0.0122

It is obvious from the values that the NMME modification is merely 2 to 4 percent.

In the Birch Scheme of equations it appears that even the parameter Bo` is quite often not contributing to the p-v relationship as the term involving Bo` occurs as multiplying factor (Bo`-4)and the Bo` values for many solids are close to four.

The NMME2 is the only equation which yields a value of the third order pressure derivative of the bulk modulus. This value turns out to be extremely small as could be anticipated but the parameter b to which Bo``` is related invariably obtains a significant value suggesting that Bo`` may not be neglected in an accurate description of the equation of state. It is therefore hoped that the values of Bo``` obtained in the present study may prove useful in studies in suitable functional forms.

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