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An Analysis of Thermodynamic Behaviour of Al and Cu at High Compressions

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Abstract

Aluminium and Copper are the pressure standard materials extensively studied and are found suitable for the purpose. The high pressures 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. The pressure-volume relationship, isothermal bulk modulus B_T and pressure derivative of B_T have been evaluated for Al and Cu down to a compression of V/V_O=0.1 using Hama and Suito equation of state. The results obtained from the Hama and Suito EOS is found to present in general fair agreement with each other for the two solids up to quite high compressions.

Keywords: EOS; Bulk modulus; Pressure derivative of bulk modulus.

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Introduction

The equation of state (EOS) of a solid describes the relationships among thermodynamic variables such as pressure, temperature, and volume. It provides numerous information of non-linear compression of a material at high pressure, and has been widely applied to engineering and other scientific researches. Recently, rapid advances in computational capabilities and accurate high-pressure experimental techniques have extremely promoted the theoretical works. Significant progress has been achieved over the past years to describe the properties of condensed matter in terms of universal relationships involving a small number of parameters. The equation of state is one of the most fundamental properties of a solid since it reveals how the volume of a sample changes under applied pressure. Even though the individual lattice parameters of a solid may decrease or increase under pressure, its volume must always decrease. At extremely high pressures, the innermost atomic states broaden

into bands and the number of valence electrons increases until ultimately the atomic shell structure is completely destroyed, leaving behind a Thomas-Fermi gas of conduction electrons. In addition, the compressibility of matter is normally reduced under pressure (lattice stiffening), i.e., the lattice Grineisen parameter is positive. A large number of phenomena occurring in high pressure experiments can be explained in simple terms from the above trends.

Generally, there are three well-known semi empirical analytic EOSs, i.e., the Murnaghan [1], Birch and Rose [2,3], or Vinet equations [4]. Especially since 1986 Rose et al. proposed that there exists a universal EOS (UEOS) being valid for all types of solids through analyzing the energy band data, a lot of forms of UEOS have been proposed with different extent of success. Among these EOSs, the Vinet equation, which can be considered to be universal for all categories of solids, has extensively been applied to various solids. Compared with the experimental observations, however, the pressure derivatives of the isothermal bulk modulus deduced from the Vinet, or Rose, equation often show some remarkable deviations [5], implying that further development of the EOS with improved performance is of necessity.

Hama and Suito [6] have developed an equation of state using the augmented plane wave (APW) method and the quantum statistical model (QSM). The Hama and Suito equation of state has been found to be successful for the whole range of pressures from low to ultra-high pressures including intermediate pressures.

Theory:

The Hama and Suito equation of state is as follows

$$P = 3B_0X^{-\frac{5}{3}}\left(1 - X^{\frac{1}{3}}\right) \times \exp\left[\frac{3}{2}(B_0' - 3)\left(1 - X^{\frac{1}{3}}\right) + \left(Z - \frac{3}{2}\right)\left(1 - X^{\frac{1}{3}}\right)^2\right]$$

where $X = \frac{V}{V0}$

and $Z = \frac{3}{8}(B_0' - 1)(B_0' + 3) + \frac{3}{2}B_0B_0'' + \frac{1}{3}$

Here B_0, B_0' and B_0'' are respectively the values of isothermal bulk modulus B and its pressure derivatives $\frac{dB}{dP}$ and $\frac{d2B}{dP2}$, at P=0.

The expression for the isothermal bulk modulus B_T is obtained by differentiating the Hama and Suito equation of state as follows

$$B_T = -V\left(\frac{\partial P}{\partial V}\right)_T$$

$$= \frac{P}{3}\left[\left\{5 + \frac{X^{\frac{1}{3}}}{1 - X^{\frac{1}{3}}}\right\} + X^{\frac{1}{3}}\left\{\frac{3}{2}(B0' - 1) + 2Z\left(1 - X^{\frac{1}{3}}\right) + 3X^{\frac{1}{3}} - 6\right\}\right]$$

An expression for the pressure derivative of bulk modulus $B_T' = \frac{dBT}{dP}$ is obtained by differentiating B_T with respect to P.

$$B_T' = \frac{B_T}{P} - \frac{1}{3} + \frac{P}{9B_T}\left[X^{\frac{2}{3}}\left\{(2Z-3) - \frac{1}{\left(1-X^{\frac{1}{3}}\right)}\right\} + 5\right]$$

Results

The pressure-volume relationship, isothermal bulk modulus B_T and pressure derivative of B_T have been evaluated for Al and Cu down to a compression of V/V_O=0.1 using Hama and Suito equation of state. The results for P, B_T and B_T' as functions of V/V_O are given below. The results obtained from the Hama and Suito EOS are found to present in general fair agreement with each other for the two solids up to quite high compressions.

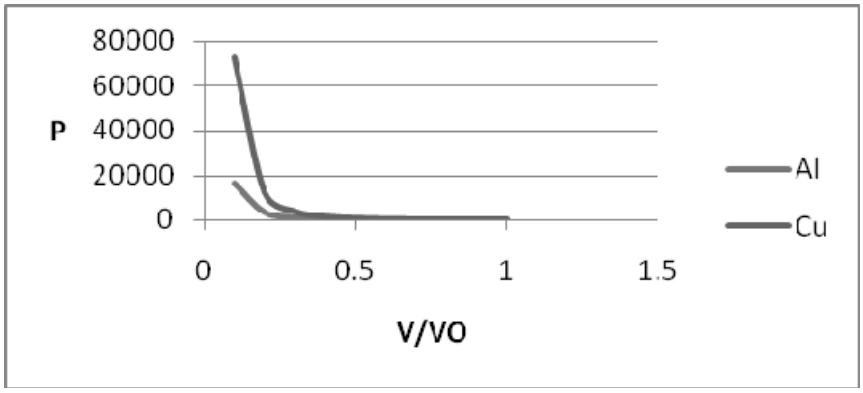

Fig1. Pressure versus relative volume for Cu and Al

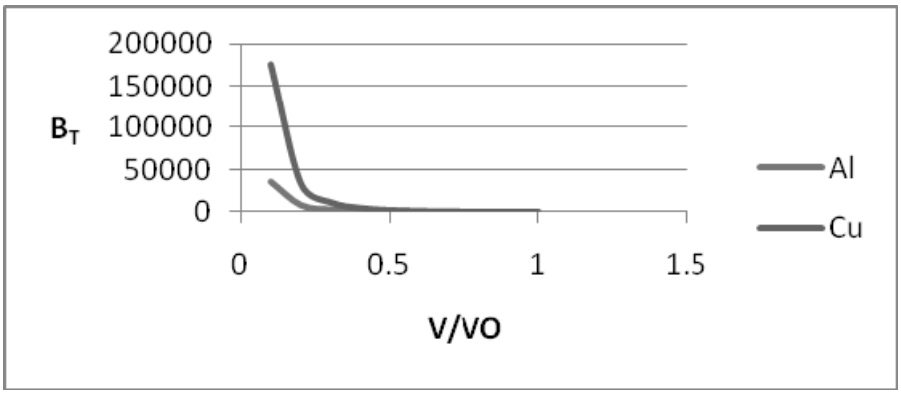

Fig2. B_T versus relative volume for Cu and Al

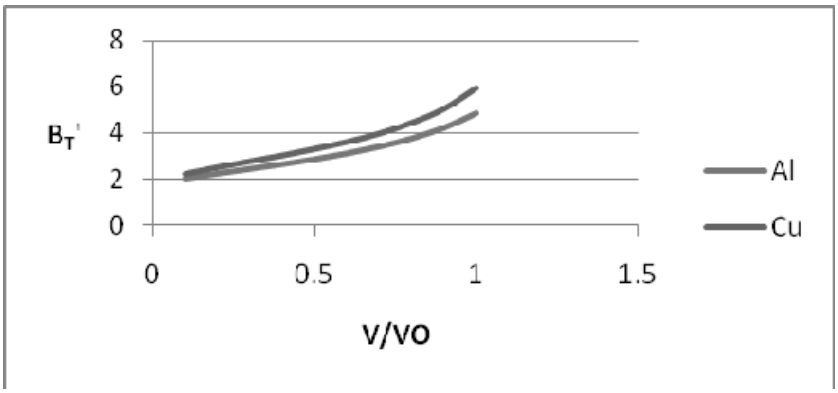

Fig3. $B_{T'}$ versus relative volume for Cu and Al

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