Publ. Astron. Obs. Belgrade No. 54 (1996), 203 – 205 *Poster*

A SIMPLE EXPRESSION FOR THE COLD COMPRESSION CURVE

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Abstract. The aim of this contribution is to present expressions for the bulk modulus of a material and its pressure derivative obtained by using the semiclassical theory of dense matter proposed by P. Savić and R. Kašanin. Some possibilities for the application of these expressions are briefly discussed.

1. INTRODUCTION

The term "equation of state" (EOS) of a system denotes any kind of relationship, established experimentally or theoretically, between the parameters of state of the system under consideration. In the particular case of a thermomechanical system, the EOS has the general form $f(p, V, T) = 0$. The knowledge of this function is of fundamental importance in various physical and astrophysical problems (for recent examples see, for instance, Holzapfel, 1996; Schulte and Holzapfel, 1996; Schaab, Weber *et al.* 1996).

A simplified version of the EOS, which does not take into account the influence of the temperature is called the cold compression curve (CCC). Strictly speaking, the CCC is a $T = 0$K isotherm of dense matter, but, in practice, it can be applied at low temperatures. In theoretical studies, the form of a cold compression curve is a consequence of the assumptions of the underlying theory (Holzapfel, 1996 contains an instructive list). One of the simplest forms of a CCC is the so-called Murnaghan EOS, which amounts to

$$P(\rho) = (B/B')[(\rho_0/\rho)^{-B'} - 1] \tag{1a}$$

In this expression, B and B' denote the isothermal bulk modulus of a material under standard conditions and its first pressure derivative. These two functions are obviously material dependent, and their knowledge is crucial for all applications of EOS. The bulk modulus is defined as

$$B = -V(\partial P/\partial V)_T = \rho(\partial P/\partial \rho)_T \tag{1}$$

The aim of this contribution is to propose simple expressions for the isothermal bulk modulus and its pressure derivative. All the calculations will be performed within a particular semi-classical theory of the behaviour of materials under high pressure, proposed by P. Savić and R. Kašanin in the early sixties (Savić and Kašanin, 1962/65). For recent reviews of their theory see Savić and Čelebonović (1994); Čelebonović (1995).

2. THE CALCULATIONS

The necessary "ingredient" for the calculation of B and B' is the function $\partial P/\partial \rho$. In the theory proposed by Savić and Kašanin this function has the following form.

$$\partial P/\partial \rho = (N_A e^2/9A)Q \tag{2}$$

where

$$Q = (4/a_i)f_i(a_i) - f_i'(a_i) \tag{2a}$$

The symbol $f_i(a_i)$ denotes the function

$$f_i(a_i) = C_i + B_i \exp(\gamma_i z_i) \tag{3a}$$

with

$$a_i = (A/8N_A\rho_i)^{1/3} \tag{3b}$$

and

$$z_i = (1 - a_i^*/a_i)/(1 - \alpha_i^{-1/3}) \tag{3c}$$

Details of derivations of these equations are avaliable in the original publications of Savić and Kašanin. The meaning of various symbols is as follows: A and N_A denote the atomic mass of the material and Avogadro's number, a_i^*, B_i, C_i, γ_i, α_i are constants (whose numerical values are known within the theory) in the i-th phase of a material subdued to high pressure. Physically, a_i is the mean inter-particle distance in the i-th phase.

Inserting eq. (3a) into (2a), it follows that

$$Q_i = (4/a_i)[C_i + B_i \exp(\gamma_i z_i)] - \gamma_i B_i \exp(\gamma_i z_i)\partial z_i/\partial a_i \tag{4a}$$

Expressing $\partial z/\partial a$ as $(\partial z/\partial \rho)(\partial \rho/\partial a)$ and using eqs. (3b) and (3c), one gets

$$\begin{aligned} Q_i =& 2(N_A\rho_i/A)^{1/3}[4(C_i + B_i \exp(\gamma_i z_i) - B_i\gamma_i(\rho_i/\rho_i^*)^{1/3} \\ & (1 - \alpha_i^{-1/3})^{-1} \exp(\gamma_i z_i)] \end{aligned} \tag{5}$$

Finally, the bulk modulus of the i-th phase of a material having the atomic mass A and density ρ is given by

$$B = 2\rho_i(N_A e^2/9A)(N_A\rho_i/A)^{1/3}[4(C_i + B_i\exp(\gamma_i z_i) - B_i\gamma_i(1-\alpha_i^{-1/3})^{-1}(\rho_i/\rho_i^*)^{1/3}\exp(\gamma_i z_i)] \tag{6}$$

The pressure derivative of B can be calculated from eqs. (1) and (2). It thus follows that

$$B' = \partial B/\partial P = (\partial/\partial P)(\rho(\partial P/\partial\rho)) = \partial/\partial P[\rho N_A e^2 Q/9A] = = 1 + \rho(N_A e^2/9A)\partial Q/\partial P = 1 + (\rho/Q)\partial Q/\partial\rho \tag{7}$$

and

$$B' \cong 1 + 8C_i N_A^{1/3}/(24C_i N_A^{1/3} + \ll 2 \gg) + \ll 3 \gg + ... \tag{8}$$

where $\ll 2 \gg$ and $\ll 3 \gg$ denote the number of terms omitted due to space limitations.

3. CONCLUSIONS

In this note we have briefly presented a theoretical algorithm for the determination of the isohermal bullk modulus and its first pressure derivative within a particular semi-classical theory of dense matter. This is a distinct advantage over the existing literature in the high-pressure field, where B and B' are usually derived by fitting the experimental p-V data to some previously chosen form of the EOS.

The results obtained in this note give the possibility of refining the models of the internal structure of cold dense astrophysical objects (such as planets satellites or asteroids) as well as theoretically following the changes of compressibility of laboratory specimen undergoing phase transitions under high pressure. Details will be published elsewhere.

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