Interpretation of p-V Isotherms of Polyvalent Metals in Terms of Pseudopotential Model

N.V. Fomin
Department of Theoretical Physics
State Technical University
Polytechnicheskaja, 29
St. Petersburg 195251, Russia

Successful applications of the Morse potential function for the theoretical explanation of p-V-T relationship and other properties of certain one-component metals have been demonstrated in several papers (1-2). However, no microscopic formulation in favor of such volume-dependent function was so far proposed.

The pair-wise interaction discussed in this work, V(R), can be written as

$$V(R) = D(x^*(1/\rho-1) - 1) \exp (x^*(1-\rho)),$$

where $\rho = R/R^*$, R = inter-atom separation, R^* = its equilibrium magnitude, and D and x^* are constants to be determined. The quantity - D, to the nearest-neighbor approximation assumed, is considered as one-pair contribution to the covalent type binding energy of a metal. Behavior of V(R) in actual region of ρ, after proper adjustment, becomes practically identical with the Morse one.

Volume (compression) dependencies of the pressure derivative of the isothermal bulk modulus and the Grüneisen parameter provided by Slater have been calculated and compared with Pastine results.

The values of adjustable pseudopotential parameters (Z, r_c), extracted from the explicit function D (Z, r_c) are

Metal	**Ag**	**Cu**	**Au**	**Zn**	**Nb**	**Mo**	**W**
Z	3	2.8	3.8	2.1	5	5.5	6
r_c/r_A	0.44	0.41	0.49	0.44	0.37	0.43	0.43

where Z = effective ion change, r_c = core radius consistent with Ashcroft's bare-ion model, and r_A = Wigner-Seitz radius.

[1] D.J. Pastine, *J. Appl. Phys.* **35**, 3407-3414 (1964).
[2] C. Malinowska-Adamska, *et al.*, *Phys. Stat. Sol. (b)* **115**, 335-345 (1983).