

Reprinted from JOURNAL OF APPLIED PHYSICS, Vol. 34, No. 8 2330-2336, August 1963
 Copyright 1963 by the American Institute of Physics
 Printed in U. S. A.

Compressibility of Solids and Liquids at High Pressures

MELVIN A. COOK AND LEO A. ROGERS*

Institute of Metals and Explosives, University of Utah, Salt Lake City, Utah

(Received 30 November 1962)

An equation for compressibility (identical in form to the Tait equation) derived previously from the virial theorem and the Fermi-Thomas atomic model is modified on the assumption that one of its parameters ($\alpha\beta_0$) is reciprocally related to the internal pressure when the cohesive energy density is assumed to be an essential part of the internal pressure. Pressure-volume data for about fifty homonuclear solids, two alloy systems, twenty ionic compounds, and five secondary bonded liquids are analyzed and the model found to fit with surprising accuracy when due consideration is given to pressure-induced phase or polymorphic changes and thermodynamic "holes" (most important near, and above, the melting point) that may contribute appreciably to specific volume. Data from static and shock methods of compression are considered and the differences noted. The model is apparently applicable to the compression of homonuclear solids and liquids, if indeed not all condensed materials in general.

INTRODUCTION

BY application of the virial theorem and the Fermi-Thomas model, the following equations were derived¹ for thermal expansion and compressibility of homonuclear solids:

$$\alpha/3 = \alpha' = C_v/2\bar{T}_1, \quad (1)$$

$$\beta = 9R(M/\rho)^{1/3}N^{1/4}/4\bar{T}, \quad (2)$$

where α =bulk thermal-expansion coefficient, α' =linear thermal-expansion coefficient, β =compressibility, \bar{T} =average effective kinetic energy, \bar{T}_1 =average kinetic energy in the valence orbital, C_v =heat capacity, R =bond

distance, ρ =density, M =atomic weight, and N =Avogadro's number. The basic idea was simply that the Fermi-Thomas (or particle in a box) model, which implies a definite relationship between the average kinetic energy and the density [$\bar{T}=f(\rho)$], could be used to describe changes in solids. Thus, in treating thermal expansion the energy

$$H = \int_0^T C_v dT$$

was considered to lower the average kinetic energy by H . Since the total energy E is negative, a positive energy H decreases $|E|$. The virial theorem was used to relate \bar{T} and E . For compressibility, on the other hand, the work of compression should increase \bar{T} by $-(\frac{3}{2})RFN$, where F is the average force applied on each of the bonds.

The theory was considered to explain only the contribution to density changes from lattice parameter changes, and did not include those changes attributed to thermodynamic defects. For example, the contribu-

* Present address: Corning Glass Works, Corning, New York. This article comprises part of the dissertation submitted by Leo A. Rogers to the Graduate School, University of Utah in partial fulfillment of the requirements for the Doctor of Philosophy degree, June 1962.

¹ M. A. Cook, Discussions Faraday Soc. 22, 203 (1956); "Properties of Solids," Bulletin No. 53, University of Utah, September 1951; J. Appl. Phys. 30, 725 (1959); *The Science of High Explosives* (Reinhold Publishing Corporation, New York, 1958), Chap. 9.