

THE COMPRESSIBILITY OF METALS

M. B. Gitis

A. A. Zhdanov Leningrad State University

Translated from *Fizika Tverdogo Tela*, Vol. 9, No. 4,

pp. 1183-1186, April, 1967

Original article submitted October 13, 1966

Experimental results indicate that the temperature coefficient of the compressibility of metals is larger in the solid state than in the liquid state, although the bulk expansion coefficient α in the solid metal is significantly less than in the liquid metal. It is shown that this effect can be related to the nonuniform volume distribution of the valence electron gas density in solid metals. A transformation from a nonuniform to a uniform distribution increases the temperature coefficient of the compressibility and decreases α .

Investigations of the temperature dependence of the compressibility β in metals in the solid [1] and liquid [2] state have shown that the temperature coefficient of the compressibility in the solid metal is somewhat greater than in the liquid, although according to theory [3] the increase of β with temperature is related to an increase of the interatomic distance, i.e., $(1/\beta)(d\beta/dT) \sim \alpha$ (α is the temperature coefficient of the volume expansion), while $\alpha_{\text{sol}} < \alpha_{\text{liq}}$. The indicated experimental fact is probably not fully accounted for by the change of the carrier effective mass with temperature, or by various types of structural transformation, since it is observed in all metals which have been studied, including alkali and noble metals (for example silver) in which heating is not accompanied by these features. Evidently this effect is related to the presence in all solid metals of a nonuniform distribution of charge density. In [4] it was shown how taking the screening of the valence electrons into account within the framework of perturbation theory leads to an increase of the wave function in the region R_0 ($2R_0$ is the distance between the centers of ions). In the Wigner-Seitz approximation this is equivalent to assuming that in the peripheral regions of the elementary sphere the density of the valence electron gas is $\rho_1 + \delta\rho$ (ρ_1 is the density over the remaining part of the sphere). From very general arguments one can conclude that the intensification of the thermal motion of the ions on heating leads to a more uniform distribution of the electron density. In liquid metals, due to the absence of long-range order, the density of the valence electron

gas is practically uniform immediately after melting [5].

We can show that this mechanism leads to an increase in the temperature coefficient of the compressibility in a solid metal in comparison to the liquid. Actually, if $(T/\beta)(\partial\beta/\partial T)_V \ll 1$ we have for the isothermal compressibility

$$\frac{1}{\beta} = V \left(\frac{\partial^2 U}{\partial V^2} \right)_T. \quad (1)$$

Here U is the internal energy of the metal and V is the volume.

The construction of a rigorous quantum theory of the cohesive forces in a metal encounters a whole series of difficulties; therefore, the dependence of U on V will be estimated on the basis of the statistical theory of metals [3]. Such an approach in the present case is also quite convenient because within the framework of statistical models the difference between a liquid and a solid metal vanishes, since long-range order is not assumed. In this model the internal energy is composed of the kinetic energy of the electron gas, the electron-ion attraction energy, and the ion-ion interaction energy (the appearance of the latter term is related to the overlap of the inner electron shells of neighboring ions; this always occurs in polyvalent and noble metals). We assume that the transition to a more uniform distribution of the valence electron density does not much alter the ionic interaction, and also the depth to which the conduction electrons penetrate the electronic orbitals of the ions [3]; therefore, we will