

III. LOW TEMPERATURE PHYSICS

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A. HEXAGONAL CLOSE-PACKED METALS

A lattice calculation was carried out for monatomic, hexagonal, close-packed metals in connection with our experimental project on low-temperature elastic constants. This calculation will form the basis for using the elastic constants at 0°K to obtain the frequency spectrum of normal modes of vibration of the lattice, $g(\nu)$. This frequency spectrum is of value in predicting and correlating such properties as specific heat, thermal expansion, and transport phenomena.

The theory comprises two parts. Part 1 provides connections between the elastic constants and a set of atomic force constants for the lattice. Part 2 utilizes these force constants in a lattice dynamical computation of the normal modes. Part 1 will be discussed here in terms of the lattice model that was adopted and the results that were obtained from room-temperature data. Part 2 has been completed to the point of finding the 6×6 complex secular determinant for the normal modes. Calculation of the frequency spectrum will be carried out on the Whirlwind computer when low-temperature force constants are available.

The model is in terms of a general axial ratio, c/a . In obtaining the potential energy of the lattice it is assumed that: (a) the displacements from equilibrium are small compared with the interatomic distance, and only harmonic terms are considered; (b) components of displacements normal to the line between equilibrium positions of the atoms do not contribute to the restoring force; thus only central forces are used. Also, the lattice forces are taken to be short range: only the interactions of an atom with the six nearest neighbors in the basal plane (Hooke's Law force constant α), the six nearest neighbors out of plane (force constant β), and the six next nearest neighbors out of plane (force constant γ) are included. The electron gas contribution to the elastic constants is assumed to arise from an isotropic volume-dependent term in the energy. Thus, there is an additive term corresponding to the bulk compressibility of the electron gas in c_{11} , c_{12} , c_{13} , and c_{33} , but not in c_{44} . This bulk compressibility, called σ , is given by the deviation from the Cauchy relation, $\sigma = c_{13} - c_{44}$.

The method of homogeneous deformation is used to find the strain energy density as a pure quadratic form in the external strain components. This permits identification of the five independent elastic constants in terms of the four lattice parameters, $\alpha, \beta, \gamma, \sigma$. If the expressions for $c_{11} + c_{12}$, c_{33} , c_{13} , and c_{44} are used to calculate these four parameters, the accuracy with which c_{11} or c_{12} can be reproduced gives some indication of the validity of the model. Values of the force constants (in dynes/cm) and σ (in dynes/cm²) are given below for magnesium and cobalt along with the calculated and experimental values of c_{11} .

(III. LOW TEMPERATURE PHYSICS)

	a	β	γ	σ	c_{11} (calc.)	c_{11} (exp.)
Mg	9.78×10^3	9.54×10^3	0.47×10^3	0.016×10^{12}	0.589×10^{12}	0.572×10^{12}
Co	45.61×10^3	46.10×10^3	-3.15×10^3	0.272×10^{12}	3.197×10^{12}	3.071×10^{12}

The agreement is fairly good for magnesium and cobalt, which have close to an ideal axial ratio and are essentially isotropic materials. The model works less well for cadmium, zinc, and beryllium, the other metals for which elastic data are available. For cadmium and zinc, the model is probably inadequate, owing to their remarkable anisotropy. A general tensor force model should be used rather than central forces. Unfortunately, the tensor force model requires 7 force constants to describe just the 12 nearest neighbors and is intractable at present. In the case of beryllium, the difficulty may come from poor elastic data.

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