# On the Elastic Constants of Polycrystalline Argon†

By C. Feldman‡ and M. L. Klein
Department of Physics, Rutgers University, New Brunswick, New Jersey, U.S.A.

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Abstract

A recent calculation of the explicit temperature dependence of the quasi-harmonic second-order elastic constants of the f.c.c. lattice with arbitrary nearest-neighbour central forces is used to calculate the bulk modulus, polycrystalline shear modulus and the polycrystalline longitudinal wave velocity for argon. The numerical calculations are based on a Mie–Lennard–Jones (12-6) potential and cover the range $0<T\lesssim 60°$K. There is reasonable agreement with available experimental data. At the highest temperatures comparison of the theoretical and experimental bulk modulus suggests that higher order anharmonic effects may be important for solid argon.

## § 1. Introduction

In the last few years a considerable number of experiments have been carried out on rare-gas solids and many of these experiments have been on polycrystalline samples. For example, Jones and Sparkes (1964) measured the resonant frequency of torsional vibration of a suspended polycrystalline rod of argon between 18 and 65°K. They were able to derive the temperature dependence of the shear modulus (or equivalently the transverse wave velocity) of the polycrystal by normalizing their data to the earlier measurements of Barker and Dobbs (1955). Lawrence and Neale (1965) obtained values for the polycrystalline longitudinal wave velocity at temperatures between 54 and 83°K using a diffraction of light technique. The isothermal bulk modulus has been measured at 4·25°K by Peterson *et al.* (1966) and at 77·7°K by Urvas *et al.* (1967), by studying the variation in the crystal lattice parameter with applied helium pressure. More recently, Moeller and Squire (1966) and Gsänger *et al.* (1967) have reported single crystal wave velocities.

In order to calculate the elastic properties of argon we need to know the interatomic forces in the solid. While there is no doubt that the dominant forces in the solid are of the central two-body type, there is increasing evidence (see, for example, the Faraday Society Discussion on Intermolecular

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‡ Present address: Grumman Aircraft Engineering Corporation, Long Island, New York, U.S.A.