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ELASTIC CONSTANTS AND CALCULATED LATTICE VIBRATION FREQUENCIES OF Mg₂Sn*

L. C. DAVIS,[†] W. B. WHITTEN[‡] and G. C. DANIELSON

Institute for Atomic Research and Department of Physics, Iowa State University, Ames, Iowa, U.S.A.

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Abstract—The longitudinal and shear sound velocities of Mg₂Sn in the [100], [110] and [111] directions have been measured between 80 and 300°K by a resonance technique. The elastic constants were computed from these velocities. Lattice vibration frequencies have been calculated for two point ion models and a shell model. Best agreement with the experimental specific heat data was obtained for the shell model, which reproduced quite accurately the sharp minimum in the Debye temperature near 20°K.

INTRODUCTION

 Mg_2Sn IS A II–IV compound semiconductor with the fluorite structure and is a member of the family of compounds Mg_2X , where X can be Si, Ge, Sn, or Pb. The elastic constants and calculated lattice vibration frequencies have been reported for Mg_2Si by WHITTEN *et al.*⁽¹⁾ and for Mg_2Ge by CHUNG *et al.*⁽²⁾ The present investigation was undertaken to extend our knowledge of the elastic properties of the Mg_2X family to include Mg_2Sn .

The reststrahl frequency and high and low frequency dielectric constants of Mg₂Sn have been measured by KAHAN *et al.*⁽³⁾ Just as in the cases of Mg₂Si⁽¹⁾ and Mg₂Ge,⁽²⁾ it seemed feasible to calculate the lattice vibration frequencies from these optical constants and the elastic constants which we could measure. In addition to the two point ion models described by CHUNG *et al.*,⁽²⁾ a new model which takes into account the polarizability of the Sn ions can be used. The calculated specific heat of the three models can then be compared to the experimental data of JELINEK *et al.*⁽⁴⁾

The phonon dispersion curves are important for an interpretation of the semiconducting

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† AEC Postdoctoral Fellow.

[‡] Now at Brookhaven National Laboratory, Upton, N.Y., U.S.A. properties of these compounds.⁽⁵⁻⁷⁾ Piezoresistance measurements have shown that the energy minima lie along the $\langle 100 \rangle$ axes in Mg₂Si⁽⁸⁾ and in Mg₂Sn.⁽⁹⁾ Therefore, a knowledge of the phonon frequencies in the $\langle 100 \rangle$ directions is particularly important since such phonons are involved in indirect transitions between the valence band and the conduction band.

EXPERIMENTAL SOUND VELOCITIES AND ELASTIC CONSTANTS

The velocity of sound in Mg_2Sn was measured by a resonance technique. Two 10 MHz quartz transducers were bonded to opposite parallel faces on each sample. One transducer was driven by the output from an Arenberg ultrasonic oscillator, Model PG-650C, operating in the continuous wave mode. The output of the other transducer was amplified and displayed on a scope. Frequencies were measured with a Bolton Labs BC-221-AL frequency meter. The sample holder is shown in Fig. 1. Two different materials were used to bond the transducers to the sample: below 250°K, beeswax was used.

Single crystal ingots were grown by a Bridgman method. Three samples were prepared with orientations [100], [110], and [111]. The sample lengths were 0.520, 0.375 and 0.943 cm, respectively.

439