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ELASTIC CONSTANTS AND CALCULATED LATTICE VIBRATION FREQUENCIES OF Mg_2Sn*

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Abstract—The longitudinal and shear sound velocities of Mg_2Sn 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 Mg_2Sn have been measured by KAHAN *et al.*[3] Just as in the cases of Mg_2Si[1] and Mg_2Ge,[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 properties of these compounds.[5–7] Piezoresistance measurements have shown that the energy minima lie along the $\langle 100 \rangle$ axes in Mg_2Si[8] and in Mg_2Sn.[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.

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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, vacuum grease was used; and above 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.

Parallel faces on opposite ends of each sample were polished with diamond paste on a silk velvet cloth. It was found that polished faces were necessary in order to obtain clear resonances.

As the frequency of the oscillator was swept from 5 to 15 MHz, 15–25 resonances could be detected. The condition for a resonance has been given by WILLIAMS and LAMB[10] as:

$$2\pi f_n \tau - \phi_n = n\pi,$$

where $\tau = l/v$, l is the sample length and v is the velocity of sound, f_n is the resonant frequency and

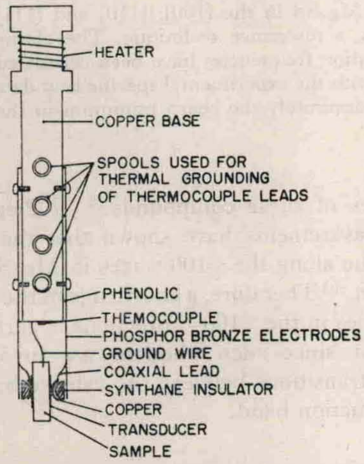

FIG. 1. Sample holder for sound velocity measurements.

ϕ_n is the phase shift which occurs when a sound wave is reflected at the sample boundary. WILLIAMS and LAMB[10] have derived an expression for ϕ_n as a function of frequency, depending upon the acoustic impedances of the sample, bonding material, and transducers, and upon the resonant frequency of the transducers (10 MHz in this case). However, it was found experimentally that for Mg_2Sn, ϕ_n was nearly frequency independent except near 10 MHz where we expected a phase shift of 180° as the frequency was passed through the fundamental of the transducers.

In the region where ϕ_n is independent of frequency, the velocity of sound is given by:

$$v = 2l\,\frac{df_n}{dn}$$

As a check, measurements were made of the velocity of sound in Ge and compared to the values of MCSKIMMIN.[11] It was found that shear measurements agreed to within 1 percent and longitudinal measurements to within 2 percent over the temperature range 77–300°K.

The velocity of sound in Mg_2Sn is shown in Figs. 2 and 3. The solid lines in Fig. 3 were computed from the three velocities in Fig. 2, and agreed satisfactorily with the measured values. None of the velocities showed more than a 2·5 percent change between 100° and 300°K. From the sound velocities and the X-ray density of

$$3{\cdot}592\ \mathrm{g/cm^3},^{(12)}$$

the elastic constants at 300°K were calculated to be:

$$C_{11} = (8{\cdot}24 \pm 0{\cdot}33) \times 10^{11}\ \mathrm{dyn/cm^2},$$

$$C_{12} = (2{\cdot}08 \pm 0{\cdot}33) \times 10^{11}\ \mathrm{dyn/cm^2},$$

$$C_{44} = (3{\cdot}66 \pm 0{\cdot}07) \times 10^{11}\ \mathrm{dyn/cm^2}.$$

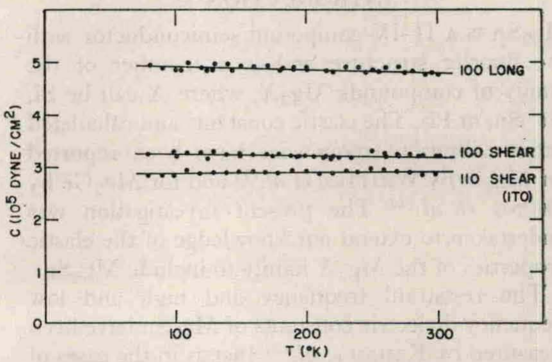

FIG. 2. Sound velocity in Mg_2Sn: [100] and [110] directions.

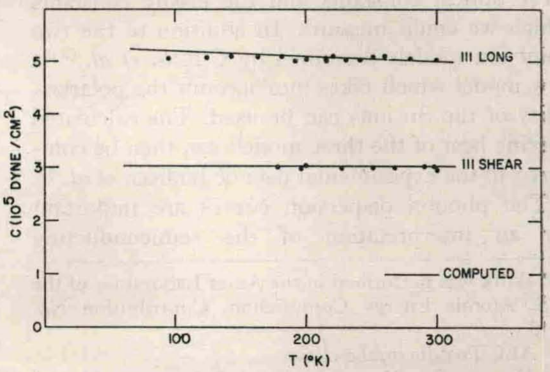

FIG. 3. Sound velocity in Mg_2Sn: [111] direction. Solid line computed from the three velocities in Fig. 2.