

imperfection elastic instability. When the crystal is cooled to below the equilibrium transformation temperature, these regions (which were previously transformed) propagate through the crystal, transforming the entire crystal to the closest packed phase. As an example, consider the core of a dislocation. Usually there is a dilatation of two atomic volumes per atom length of dislocation. A crude model assumes that linear elasticity describes the stress field of the dislocation which is postulated to be hollow. The stress field arises from the rigid displacement and the presence of an internal pressure P in the cylindrical core. If $P \approx B/6$, this model leads to the expected dilatation. For lithium the quantity $B/6$ represents a pressure of approximately 22 kbar. Although C' at $P = 0$ is not zero, there exists the possibility that dC'/dP is negative so that C' might in fact be zero at the pressure assumed to be present in the core.

1.4 Theoretical predictions of elastic constants

The pioneering work in the area of calculating the elastic properties of metals was performed in the mid-thirties by Wigner and Seitz [20 to 22], Bardeen [23] and Fuchs [24]. The latter approach yielded elastic constants other than the bulk modulus, and has been varied [25 to 28] to explain discrepancies between observed and calculated data. Since the mid-sixties an approach applying pseudopotential theory [29 to 32] has enabled theorists to calculate various properties, including the elastic constants, of the simple metals and to predict elastic constant values which agree well with recently reported experimental results.

In the present paper results are presented which show that a bulk instability does not exist. Moreover, the present evidence tends to rule out the imperfection elastic instability mechanism (but not completely). Finally, we show that the agreement between the measured pressure derivatives and theoretically predicted values at 0 °K is fair.

2. Experimental Techniques

A pulsed ultrasonic interferometer was used to measure the elastic constants of the lithium single crystals. The pulse system is described in detail elsewhere [33], as are the temperature and pressure control systems [34].

The scarcity of single crystal data on lithium metal is primarily due to the difficulty of obtaining large single crystals. Bender [35] made unsuccessful attempts to grow lithium single crystals although he was able to obtain large single crystals of both sodium and potassium. Bowers et al. [36] reported a successful method for producing small (0.63 cm diameter) cylindrical single crystals. The procedure originated by Nash and Smith [18] was used to produce the crystals for the present research.

The ultrasonic specimen preparation for lithium follows those procedures for sodium outlined by Martinson [33]. The etching and cleaning solutions used were anhydrous diethyl-ether and methyl alcohol, respectively. The final sample size was approximately $(1.5 \times 1.0 \times 1.0)$ cm³.

3. Data Analysis

The analysis of the results of the experiments (frequencies at sets of T, P) was carried out in the following manner:

1. The transit times were corrected to take into account the presence of a transducer.

2. The length l_0 at temperature T and atmospheric pressure was computed from thermal expansion data.

3. The length l at T, P was computed as described later.

4. A least square analysis was then used at each temperature with C having the linear form

$$C = C|_{P=0, T} + \left. \frac{dC}{dP} \right|_{P=0, T} P. \quad (1)$$

The equation for the transit time is

$$2\tau = \frac{n - \frac{1}{2} + p}{f_n p} + k(f_n^{-1} - f_0^{-1}), \quad (2)$$

where 2τ is the round trip transit time of the sample, f_n is the frequency at which interference occurs, n is an integer associated with the frequency f_n , p is the difference between the number of round trips of the two pulses, k is the ratio of the transducer to sample acoustic impedances, and f_0 is the free resonance frequency of the transducer. The elastic constant is calculated from the following formula:

$$C = \rho \frac{l^2}{\tau^2}, \quad (3)$$

where ρ and l are the sample density and length, respectively. The temperature and pressure variation of the resonance frequency of the transducer are taken from McSkimin and Andreatch [37] and the length change variation of the lithium sample with temperature is from Pearson [38]. Cook's analysis [39] was used to evaluate the length change of the sample resulting from the application of hydrostatic pressure. This involved the calculation of the conversion factor Δ at temperature and pressure. The specific heat data of Martin [40] was used in addition to Pearson's data to calculate Δ as defined by

$$\Delta = \frac{\beta^2 B^S T}{\rho C_P}, \quad (4)$$

where β is the volume thermal expansion coefficient, C_P is the heat capacity at constant pressure, B^S is the adiabatic bulk modulus, and T is the absolute temperature.

4. Results

Transit time measurements were made which resulted in values of

$$C' = (C_{11} - C_{12})/2, C_{11}^S, \text{ and } C_n^S = C_{11}^S - C' + C_{44}.$$

The values of C_{44} , B^S , and B^T were calculated from the three measured constants using the well-known relations

$$C_{44} = C_n^S - C_{11}^S + C', \quad (5)$$

$$B^S = C_{11}^S - \frac{4}{3} C', \quad (6)$$

and

$$B^T = \frac{B^S}{1 + \Delta}.$$