Variation of the Elastic Constants of Li with Temperature and Pressure

Table 1

Table 1 presents the results of the analysis of the data for C_{11}^S , and C_n^S and C' evaluated at 100 °K, as well as the constants C_{44} , and B^S and B^T which have been computed from the measured values.

Two other sets of atmospheric pressure ultrasonic data are available [18, 19]. These and the present absolute values evaluated at 100 °K are itemized in Table 2.

Table 3 compares the results of three calculations (Fuchs [24], Boffey [25], and Suzuki et al. [30]) with the three sets of absolute value data extrapolated to T = 0 °K. In the case of the Nash and Smith data, where only three temperature points were taken, the extrapolation is somewhat more uncertain than for either of the other two sets.

Table 4 contains a summary of temperature derivatives. The present data agrees most often with that published by Slotwinsik and Trivisonno [19]. This would reasonably be the case as the number of points used to determine the slope in that data is large compared to the number of points for the Nash and Smith data.

Swenson [41], on the basis of direct PVT measurements, obtained a value of $\mathrm{d}B^T/\mathrm{d}T = -5 \times 10^{-2} \mathrm{\,kbar/deg\ contrasted}$ to the present value of -6×10^{-2} kbar/deg.

The zero temperature extrapolated pressure derivatives are compared with those derived theoretically by Suzuki et al. [30], in Table 5. The Suzuki data was calculated using a core radius value of 1.36 at. units. Using a value of 0.92 at. units the agreement between the calculated and experimental pressure derivatives is much better but the values of the calculated elastic constants are changed greatly by this choice of core radius.

Table 6 compares the pressure derivatives of the shear constants C' and C_{44} given by Jain [27] with the present results. The agreement is very good.

The values of B_0^T and $(dB_0^T/dP)_T$ obtained by various methods are summarized in Table 6.

The shock values are obtained from Rice's [42] measured values of c and s in the rela-

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	Results of	curve fitting tem	perature and pre-	ssure data		
	C_{11}^S	C_n^S	C,	C_{44}	B^S	B^{T}
= 100 °K = 0 kbar	142.3 ± 0.7	238.0 ± 0.9	11.3 ± 0.02	107.0 ± 0.9	127.2 ± 0.7	126.5 ± 0.7
10^{-2} kbar deg ⁻¹) = 0 kbar	-4.75 ± 0.2	-14.1 ± 0.4	-0.42 ± 0.02	-9.8 ± 0.5	-4.2 ± 0.2	-6.0 ± 0.2
dimensionless) = 100 °K	3.44 ± 0.1	4.36 ± 0.2	0.06 ± 0.01	0.98 ± 0.2	3.36 ± 0.1	3.38 ± 0.1
$\mathrm{d}P~(\mathrm{deg}^{-1})$	0.08 ± 0.09	0.12 ± 0.17	0.01 ± 0.005	0.05 ± 0.26	0.07 ± 0.10	0.09 ± 0.10
$dP \ (\deg^{-1})$	0.08 ± 0.09	0.12 ± 0.17	0.01 ± 0.005	$0.05\pm$	0.26	0.26 0.07 ± 0.10

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Table 2

Values of elastic constants from various sources. Units of kbar, T = 100 °K, P = 0 kbar

C_{11}^{S}	C_n^S	C'	C44	B^S	reference
146.0	240.3	11.5	105.8	130.7	[18]
143.5	239.4	11.0	107.3	128.8	[19]
142.3	238.0	11.3	107.0	127.2	present paper

Table 3

Experimental and theoretical values of elastic constants *) from various sources. Units of 10^2 kbar, T = 0 °K, P = 0 kbar

	C ₁₁	Cn	<i>C</i> ″	C44	В	reference
(calc)	1.53	2.69	0.17	1.33	1.30	[24]
(calc)	1.50	2.54	0.12	1.16	1.34	[30]
(calc)			0.11	1.11		[25]
(exp)	1.54	2.55	0.119	1.13	1.38	[18]
(exp)	1.47	2.49	0.112	1.13	1.32	[19]
(exp)	1.46	2.48	0.116	1.14	1.31	present paper

*) Adiabatic and isothermal elastic constants and bulk moduli are equal at T = 0 °K.

Table 4

Temperature derivatives of elastic constants from various sources evaluated at 300 °K. Units of 10^{-2} kbar deg⁻¹, P = 0 kbar

$\mathrm{d}C_{11}^S/\mathrm{d}T$	$\mathrm{d} C_n^S/\mathrm{d} T$	$\mathrm{d}C'/\mathrm{d}T$	$\mathrm{d}C_{44}/\mathrm{d}T$	$\mathrm{d}B^S/\mathrm{d}T$	reference
-11.8 - 4.7 - 4.75	$-21.5 \\ -13.7 \\ -14.1$	$-0.6 \\ -0.3 \\ -0.42$	$-10.3 \\ - 9.3 \\ - 9.8$	-11.0 - 4.3*) - 4.2	[18] [19] present paper

*) Value tabulated in Table 2 of [19] is -3.1 but this appears to be in error.

tion $u_{\rm s} = c + s u_{\rm p}$, where

$$c = \left(\frac{B_0^S}{\varrho_0}\right)^{1/2} \quad \text{and} \quad s = \frac{1}{4} \left[\left(\frac{\mathrm{d}B_0^S}{\mathrm{d}P}\right)_S + 1 \right],\tag{7}$$

and u_s and u_p are the shock and particle velocities, respectively. The adiabatic quantities are then converted to isothermal quantities. The results for both B_0^T and (dB_0^T/dP) at 300 °K are good (Table 7).

5. Discussion

One motivating force of the present work was the desire to test the validity of 1. the bulk elastic instability concept proposed by Zener for b.c.c. metals, and 2. a microscopic elastic instability argument, as possible mechanisms for martensitic-type transformations. None of the three sets of data indicate a bulk elastic instability. All room pressure elastic constants have negative temperature