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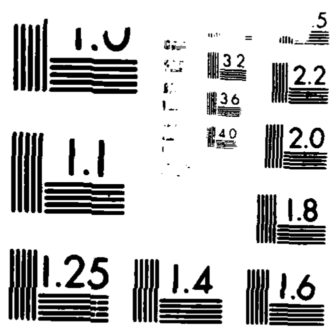
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TECHNICAL REPORT ARCCB-TR-86018

THE ELASTIC CONSTANTS OF Ni_3Al TO 1.4 GPa

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MAY 1986

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The pressure derivatives of the elastic constants of single-crystal Ni_3Al have been determined to 1.4 GPa by both pulse superposition and pulse-echo overlap techniques. Measurements were made on single-crystal specimens of orientation <100> and <110>, thus providing at least one cross-check. The values of c_{11}, c_{12}, and c_{44} at one atmosphere are found to be 223.5, 149.0, and 122.9 GPa, respectively. The pressure derivatives of the elastic constants have been determined.

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INTRODUCTION

Ni_3Al, having the $L1_2$ ordered structure, belongs to a class of intermetallic compounds which shows unusual mechanical behavior, namely, a peak in mechanical strength with an increase in temperature. The peak temperature for Ni_3Al is 922 K, where the yield stress value is four times its value at room temperature. A large number of investigations determining the dependence of different physical properties as a function of temperature have been done, but the pressure dependence of the properties of Ni_3Al remains to be investigated in depth. The present report fills this gap in our information by determining the pressure dependence of the three elastic constants c_{11}, c_{12}, and c_{44} of single-crystal Ni_3Al to 1.4 GPa at room temperature. The results of the present investigation are compared with previous elastic constant measurements at ambient conditions reported by Dickson et al. (ref 1) and Ono and Stern (ref 2). Our results are also compared with diffraction data to 12.0 GPa developed by Mauer et al (ref 3).

EXPERIMENTAL DETAILS

A single-crystal ingot of Ni_3Al was generously provided by Dr. B. H. Kear of United Technologies Research Center, Connecticut. Two nearly cubical specimens of Ni_3Al, one having [100] type faces and the other having two pairs of [110] and one pair of [100] type faces, were prepared from the crystal

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[1] R. W. Dickson, J. B. Wachtman, Jr., and S. M. Copley, J. Appl. Phys., Vol. 40, 1969, p. 2276.
[2] K. Ono and R. Stern, Trans. Met. Soc. AIME, Vol. 245, 1971, p. 171.
[3] F. A. Mauer, R. G. Munro, G. J. Piermarini, S. B. Block, and D. P. Dandekar, J. Appl. Phys. (to be published).

ingot. The faces on these specimens were oriented normal to ± 0.5 degree of their respective crystallographic directions by the back-reflection Laue technique. The parallel faces were hand-lapped, etched, and polished by the usual metallographic procedure. The specimen having only [100] type of faces had a thickness of 0.9525 ± 0.0005 cm. The thicknesses of the [110] type faces on the second specimen were 0.970 and 0.951 cm, respectively. The density was determined to be 7.478 ± 0.007 Mg/m^3.

The values of the three elastic constants c_{11}, c_{12}, and c_{44} were obtained from measurements of travel times of longitudinal and shear waves in the <100> and <110> directions. Two independent sets of these measurements were performed on the two specimens. One set of measurements was done at the University of Chicago. The second set of measurements was made at Benet Weapons Laboratory.

At the University of Chicago, the acoustic velocities were measured using the pulse superposition method developed by McSkimmin (ref 4). X and AC cut quartz transducers with a fundamental frequency of 30 MHz were used to generate longitudinal and shear modes, respectively. They were bonded to the crystals by using DOW 276-V9 resin. The pulse repetition frequencies were recorded. A Bridgman pressure vessel was used, and pressure was determined using a calibrated Manganin coil. Measurements were performed to 0.6 GPa. The error in the absolute value of a velocity is estimated to be less than 0.5 percent. Relative accuracy is much greater.

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[4]H. J. McSkimmin, J. Acoust. Soc. Am., Vol. 33, 1961, p. 12.

At Benet Weapons Laboratory, the acoustic velocities were measured to 1.4 GPa with the pulse-echo overlap method of Papadakis (ref 5) using a two frequency approach. Simply put, the experiment is done twice--once with a 10 MHz (for example) and once with a 15 MHz transducer. The result of the cycle-for-cycle comparison should be the same at the two transducer frequencies, but only if the correct cycle is chosen.

DATA ANALYSIS

The values of the elastic constants were estimated by the method of least squares from the pulse repetition or pulse-echo overlap frequencies measured for four acoustic modes. They are longitudinal in <100> and <110> directions, shear in <100> and shear in <110> polarized along $\langle\bar{1}10\rangle$. For these modes in a cubic crystal we have

$$\rho V_\ell^2\langle 100\rangle = c_{11} \equiv K_1 \tag{1}$$

$$\rho V_s^2\langle 100\rangle = c_{44} \equiv K_2 \tag{2}$$

$$\rho V_\ell^2\langle 110\rangle = (c_{11}+c_{12}+2c_{44})/2 \equiv K_3 \tag{3}$$

$$\rho V_s^2\langle 110\rangle p\langle\bar{1}10\rangle = (c_{11}-c_{12})/2 \equiv c_s \equiv K_4 \tag{4}$$

We can construct a function F

$$F \equiv (K_1-c_{11})^2+(K_2-c_{44})^2 + (K_3-0.5c_{11}-0.5c_{12}-c_{44})^2+(K_4-0.5c_{11}+0.5c_{12})^2 \tag{5}$$

This function yields the least squares estimates of the three elastic constants

$$c_{11} = (3K_1-K_2+K_3+K_4)/4 \tag{6}$$

---

[5]E. P. Papadakis, J. Acoust. Soc. Am., Vol. 42, 1967, p. 1045.

$$c_{12} = (K_1-3K_2+3K_3-5K_4)/4 \quad (7)$$

$$c_{44} = (-K_1+3K_2+K_3+K_4)/4 \quad (8)$$

Equations (6) through (8) are used to calculate the best values of the three elastic constants of Ni_3Al.

The pulse repetition and pulse-echo overlap frequencies for all four modes were found to vary linearly with pressure. Therefore, the frequency estimates for each of the modes at a given pressure were obtained from the least squares fit of a straight line for each mode. These estimates were utilized in conjunction with the estimating procedure of the elastic constants of a cubic crystal at high pressure developed by Dandekar (ref 6).

RESULTS AND DISCUSSION

The values of the elastic constants of Ni_3Al as obtained in the present investigation are given together with the previous measurements in Table I. This table shows that the values of the elastic constants of Ni_3Al obtained from the present two sets of independent measurements are in excellent agreement. On the other hand, the values of the elastic constants obtained by Dickson et al. (ref 1) and Ono and Stern (ref 2) are consistently lower than the values obtained in the present work. These differences are too large to be attributed to measurement errors in the acoustic velocities. The likely reasons for the differences in the values of the elastic constants determined by the previous workers and in the present work may be as follows. Dickson et

[1] R. W. Dickson, J. B. Wachtman, Jr., and S. M. Copley, J. Appl. Phys., Vol. 40, 1969, p. 2276.
[2] K. Ono and R. Stern, Trans. Met. Soc. AIME, Vol. 245, 1971, p. 171.
[6] D. P. Dandekar, J. Appl. Phys., Vol. 41, 1970, p. 667.

al. (ref 1) obtained the values of the elastic constants by measuring resonance frequencies of seven rods of single-crystal Ni_3Al, with different orientations and different densities. The densities of these rods varied between 7.552 and 7.582 Mg/m^3. These rods were of lengths between 10.7 and 13.8 cm and their diameter varied between 0.47 and 0.57 cm. The orientations of these rods were determined by using the Laue back-reflection technique. Even though both the ultrasonic method and the resonance technique should yield identical or very nearly identical values for the elastic constants of a solid, it is possible that different values of the elastic constants of Ni_3Al were obtained from the two techniques because the entire length of the rods used by Dickson et al. (ref 1) may not have been oriented uniformly with respect to the measurement orientation at a given point. The differences between the values of the elastic constants as obtained by Ono and Stern (ref 2) and in the present work are more difficult to explain because both sets of measurements were done on small oriented specimens by ultrasonic techniques. However, whereas the results of Ono and Stern (ref 2) cannot be checked for their internal consistency because they measured only three acoustic modes in <110> orientation of Ni_3Al, the results of the present work can be checked for their internal consistency because four independent wave velocities were measured at each of the two laboratories mentioned earlier by two different methods and different research personnel. Thus, we believe that the values of the elastic constants of Ni_3Al obtained in the present work are the valid ones.

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[1]R. W. Dickson, J. B. Wachtman, Jr., and S. M. Copley, J. Appl. Phys., Vol. 40, 1969, p. 2276.
[2]K. Ono and R. Stern, Trans. Met. Soc. AIME, Vol. 245, 1971, p. 171.

The pulse repetition frequencies and pulse-echo overlap frequencies for the four acoustic modes in Ni_3Al were found to vary linearly with pressure. The worst correlation coefficient between the frequencies and pressure was for the shear wave propagating along <110> and polarized along <$\bar{1}$10> which has a value of 0.989. The slopes of change in frequencies with pressure for the four acoustic modes measured in this work are given in Table II. The consistency between the two sets of measurements taken on the same specimens is self-evident. The pressure derivatives of the adiabatic elastic constants of Ni_3Al are given in Table III.

Compression data of Ni_3Al obtained by the in situ high pressure x-ray diffraction technique to 12.0 GPa by Mauer et al. (ref 3), showed excessive scatter. As a result they were unable to obtain an estimate for the pressure derivative of the isothermal bulk modulus of Ni_3Al. Their estimate of the isothermal bulk modulus was 185 GPa, as compared to a value of 169 GPa obtained here. The present work allows us to compute the pressure derivative of the isothermal bulk modulus B_T of Ni_3Al as 4.88. Here we have used $B_T = B_s/(1+\Delta)$ with $\Delta = \alpha\gamma T$, where $\gamma = 2.12$ is the Gruneisen constant at ambient pressure and temperature and $\alpha = 4.24 \times 10^{-5}$/K is the temperature coefficient of linear expansion. $B_s = (c_{11}+2c_{12})/3$ is the adiabatic bulk modulus. If the compression curve of Ni_3Al is expressed by Bridgman's equation $\partial V/V = aP+bP^2$, we obtain

$$-\partial V/V = 5.915 \times 10^{-3}\,P - 1.0286 \times 10^{-4}\,P^2 \qquad (9)$$

[3]F. A. Mauer, R. G. Munro, G. J. Piermarini, S. B. Block, and D. P. Dandekar, J. Appl. Phys. (to be published).

where $\partial V/V_0$ is the change in volume with respect to the ambient volume and P is pressure in GPa.

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1. R. W. Dickson, J. B. Wachtman, Jr., and S. M. Copley, J. Appl. Phys., Vol. 40, 1969, p. 2276.

2. K. Ono and R. Stern, Trans. Met. Soc. AIME, Vol. 245, 1971, p. 171.

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5. E. P. Papadakis, J. Acoust. Soc. Am., Vol. 42, 1967, p. 1045.

6. D. P. Dandekar, J. Appl. Phys., Vol. 41, 1970, p. 667.

TABLE I. DENSITY ρ (IN Mg/m^3), ELASTIC CONSTANTS c_{ij} AND ADIABATIC BULK MODULUS B_s (IN 10^{11} N/m^2) OF Ni_3Al

Source	c_{11}	c_{12}	c_{44}	B_s	ρ
Ref (2)	1.978	1.265	1.178	1.503	7.491
Ref (1)	1.688	0.886	1.212	1.153	7.563
U. of Chicago	2.232	1.495	1.228	1.740	7.478
Benet Labs.	2.238	1.485	1.230	1.736	7.478

TABLE II. SLOPES OF CHANGE IN FREQUENCY WITH PRESSURE (IN Hz/GPa) FOR VARIOUS VELOCITY MODES IN Ni_3Al

Propagation Direction	Particle Motion	Univ. of Chicago	Benet Laboratory
<100>	<100>	0.3364×10^4	0.3308×10^4
<100>	⊥ to <100>	0.1869×10^4	0.1813×10^4
<110>	<110>	0.3938×10^4	0.3825×10^4
<110>	$\langle\bar{1}10\rangle$	0.7112×10^3	0.5917×10^3

TABLE III. PRESSURE DERIVATIVE OF THE ELASTIC CONSTANTS OF Ni_3Al

Elastic Constant	Pressure Derivative
c_{11}	5.58
c_{12}	4.72
c_{44}	2.34
c_s	0.43
B_s	5.01
B_T	4.88

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