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1989 J. Phys.: Condens. Matter 1 5357

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The high-temperature thermal expansion of Ni₃Al measured by x-ray diffraction and dilation methods

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Received 27 February 1989

Abstract. The lattice parameters of Ni₃Al have been determined accurately for the temperature range 25 to 594 °C by a high-temperature x-ray powder diffraction method. These data are used to evaluate the coefficients of thermal expansion at various temperatures. The thermal expansion of Ni₃Al has also been measured from 25 to 1000 °C by a dilation method. The thermal expansion values obtained by the dilation method are in good agreement with those determined by the x-ray diffraction method at around room temperature, but the agreement deteriorates with increase in temperature.

1. Introduction

The intermetallic compound Ni₃Al (γ' -phase), which has L1₂-type structure, is of interest because of its high-temperature structural applications. The strength of the material increases with temperature up to 600 °C and the material is ordered up to its melting point (1390 °C). The alloy exhibits oxidation resistance in air at elevated temperatures, forming adherent aluminium oxide films (Liu and Stiegler 1984). Various physical properties of Ni₃Al have been studied (Dickson *et al* 1969, Kayser and Stassis 1981, Mishima *et al* 1985, Williams *et al* 1986). The thermal expansion of Ni₃Al with additions has also been studied, by the dilation method (Arbuzov and Zelenkov 1964a,b, Maniar and Bridge 1972). Arbuzov and Zelenkov observed a reduction in the coefficient of thermal expansion (α) between 480 and 550 °C while Maniar and Bridge observed a linear variation with temperature. To resolve the discrepancies in the published data on expansion characteristics, and also as part of our laboratory's ongoing programme of research into the thermal expansion of intermetallics, we have studied Ni₃Al by both x-ray diffraction and dilatometry methods.

2. Experimental details

The alloy was prepared by arc melting under an argon atmosphere using 99.9% purity elements. The button of alloy was homogenised at 1000 °C for 60 h and furnace cooled. Metallographic examination showed the alloy to be single-phase. A dilatometer sample

Table 1. A comparison of room-temperature microhardness values for Ni₃Al.

Reference	Microhardness (kg mm ⁻²)
Alexander and Vaughan (1937)	238
Kinsey and Stewart (1951)	265
Guard and Westbrook (1959)	210
Present study	250

Table 2. A comparison of room-temperature lattice parameters of Ni₃Al.

Reference	Lattice parameter (nm)
Bradley and Taylor (1937)	0.35665
Taylor and Floyd (1952)	0.35675
Guard and Westbrook (1959)	0.35700
Aoki and Izumi (1976)	0.35645
Naguchi <i>et al</i> (1981)	0.35710
Mishima <i>et al</i> (1985)	0.35700
Present study	0.35718 ± 0.00002

of length 1 in and diameter $\frac{1}{4}$ in was cut out of this button. The filings were collected from the button for x-ray study. The bulk specimen and the filings were encapsulated in separate quartz tubes under 10^{-5} Torr vacuum and annealed at 900 °C for 2 h and 24 h respectively, to relieve the stresses.

The experimental techniques and computational procedure used in the determination of the lattice parameters at different temperatures have been described earlier (Bhaskara Sastry *et al* 1987). Powder photographs were taken at seven different temperatures ranging from 25 to 594 °C using a Unicam 19 cm high-temperature powder camera and Cu K α radiation. The temperature could be controlled to within ± 2 °C. Four reflections, (331) _{α_1} , (331) _{α_2} , (420) _{α_1} and (420) _{α_2} , in the Bragg angle region from 68 to 76° were used to determine the lattice parameter at each temperature, employing Cohen's least-squares method (Cohen 1935). Independent measurements and calculations were made for several films and the average of the deviations of the values for the individual films from the mean was found to be about 0.000 02 nm.

An Orton dilatometer was used to obtain the data on the coefficients of thermal expansion of the bulk specimen up to 1000 °C. The sample was heated at the rate of 2.5 °C min⁻¹ under 10^{-5} Torr vacuum.

The microhardness of the alloy was also determined by Vicker's method using a load of 100 g.

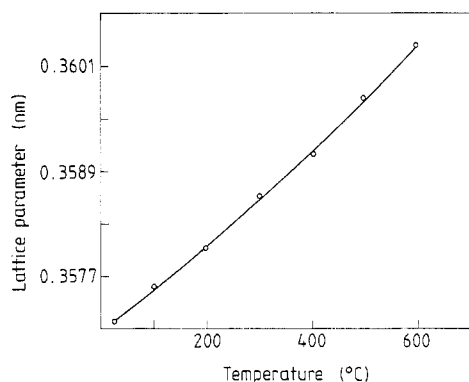
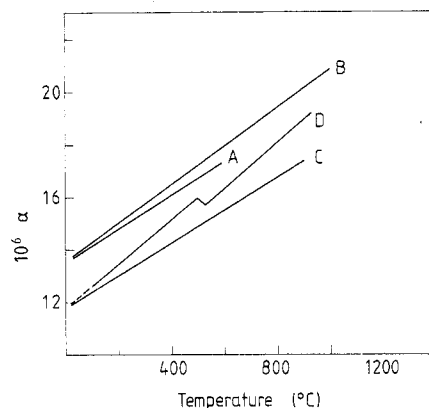
3. Results and discussion

The room-temperature hardness value obtained in the present work is in good agreement with the reported values (table 1).

In table 2, the lattice parameter of Ni₃Al obtained at room temperature is compared with the data available in the literature. Discrepancies among the lattice parameter data

Table 3. The variation of the lattice parameter of Ni₃Al with temperature.

Temperature (°C)	Lattice parameter (nm)
25	0.35718
101	0.35759
198	0.35805
300	0.35862
402	0.35921
494	0.35974
594	0.36035

**Figure 1.** The temperature variation of the lattice parameter of Ni₃Al.**Figure 2.** The temperature dependence of the coefficient of thermal expansion of Ni₃Al. Key to curves: A, present study (x-ray); B, present study (dilatometer); C, from Maniar and Bridge (1972); D, from Arbuzov and Zelenkov (1964a,b).

can be observed. They may arise from variation in the composition and also from differences between the heat treatments applied (Baker *et al* 1988).

The lattice parameters of Ni₃Al obtained at various temperatures are given in table 3 and shown in figure 1. The temperature dependence of the lattice parameter is represented by the following equation:

$$\ln a_T = -1.02983 + 1.3553 \times 10^{-5} T + 3.1424 \times 10^{-9} T^2 \quad (1)$$

where T is the temperature in °C and a_T is in nm. In figure 2 data on the thermal expansions found by the x-ray and dilatometry methods are plotted.

Arbuzov and Zelenkov (1964a,b) observed a sudden drop in the coefficient of thermal expansion in the temperature range 480–550 °C, whereas in the present study the coefficient of thermal expansion is observed to vary linearly with temperature, as also reported by Maniar and Bridge (1972). Dickson *et al* (1969) observed no anomaly in the elastic constants from 10 to 850 °C. The anomaly observed by Arbuzov and Zelenkov (1964a,b) was attributed to the electron structure of the d and s levels.

The thermal expansion values obtained by the dilation method (α_b) agree reasonably well with those determined by x-ray diffraction (α_a) around room temperature and deviate at higher temperatures. A possible explanation for this is that vacancies are

created at higher temperatures. Whether or not this is truly the case can be assessed by evaluating the differences between the expansion values obtained by the dilation method and those obtained by the x-ray diffraction method. The relevant expressions for evaluating the equilibrium concentration of vacancies are given below (Touloukian *et al* 1978).

$$n/N = 3(\Delta L/L - \Delta a/a)$$

where a is the lattice parameter as measured using x-rays. The values of n/N at the various temperatures were calculated and an Arrhenius-type plot of $\ln n/N$ against $1/T$ was drawn. From the values of the slope and the intercept of this plot, the variation of n/N with temperature can be represented by the following equation

$$n/N = 0.0158 \exp(-0.20/kT).$$

From this, the equilibrium concentration of vacancies may be estimated. The value obtained at room temperature is 7×10^{-6} and the extrapolated value at the melting point is 4×10^{-3} . This explains the differences between the dilatometry and x-ray data. However, the lower value of the formation energy (0.20 eV) in Ni_3Al is intriguing, when compared with the data reported for pure metals such as Al (0.75 eV), Pb (0.53 eV), Ag (1.09 eV) and Au (0.94 eV) (Simmons and Balluffi 1961).

The Grüneisen parameter (γ) of Ni_3Al , which is a direct measure of lattice anharmonicity, was calculated using the formula

$$\gamma = \beta V / \psi^S C_p \quad (2)$$

where β is the volume expansion, V is the molar volume, ψ^S is the adiabatic compressibility and C_p is the specific heat at constant pressure. Using the value of α obtained in the present study and values of C_p and ψ^S from Kayser and Stassis (1981), γ was calculated and was found to be 1.92.

Acknowledgments

The authors are grateful to the referees for critical comments. They thank the Ministry of Defence, Government of India, for the grant of a research scheme, under which this work was carried out. They thank Dr P Rama Rao, Director, DMRL, Hyderabad, for his interest. One of us (PVMR) thanks the CSIR, for the award of a fellowship.

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