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## LETTER TO THE EDITOR

# Elastic constants of a single crystal of Cr + 2.6 at. % Al through the Néel temperature

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**Abstract.** The temperature behaviour of the elastic constants of a single crystal of Cr + 2.6 at. % Al, which displays a commensurate spin density wave–paramagnetic transition at the Néel temperature, is reported and compared with the behaviour at the incommensurate–paramagnetic transition of pure Cr. A jump-like anomaly was observed in the compressional constants of Cr + 2.6 at. % Al compared to a  $\lambda$ -type anomaly of pure Cr. As in pure Cr, the shear constant  $\frac{1}{2}(c_{11} - c_{12})$  displays a cusp-like anomaly at the Néel temperature while no anomaly was observed in the shear constant  $c_{44}$ .

Cr is an itinerant electron antiferromagnet in which the antiferromagnetic ordering is associated with an incommensurate (I) spin density wave (SDW) state that appears below the Néel temperature,  $T_N = 311$  K. The temperature variation of the single-crystal elastic constants of Cr was studied by Bolef and de Klerk (1963), Palmer and Lee (1971), van Rijn and Alberts (1983) and Muir *et al* (1987). The compressional constants  $c_{11}$  and  $c_{12}$  show large  $\lambda$ -type anomalies at  $T_N$ , the shear constant  $c_{44}$  is only slightly affected while the shear constant  $\frac{1}{2}(c_{11} - c_{12})$  shows a relatively small cusp-like behaviour at  $T_N$ .

Alloying Cr with different elements alters the electron-to-atom ratio and consequently the Fermi surface, which gives rise to considerable changes in its physical properties. It is possible, for example, to transform the ISDW state of Cr to a commensurate (C) one on alloying. Adding Al to Cr changes the transition at  $T_N$  from an ISDW–paramagnetic (P) transition to a CSDW–P one for concentration  $C \geq 2$  at. % Al (Kallel and de Bergevin 1967, Alberts 1985, Yakhmi 1987).

The polycrystalline elastic constants of Cr–Al alloys were previously studied by Alberts and Lourens (1984) who observed well defined anomalies in the bulk modulus ( $B$ ) at  $T_N$  but not for the shear constant ( $G$ ). As in pure Cr,  $\lambda$ -type anomalies were observed in alloys having CSDW–P transitions.

The single-crystal elastic constants of Cr alloys that display CSDW–P transitions at  $T_N$  have not been studied previously. We report here measurements on a single crystal of Cr + 2.6 at. % Al. In addition to ‘jump-like’ transitions in the compressional constants  $c_{11}$  and  $c_{12}$ , a cusp-like anomaly was observed in the shear constant  $\frac{1}{2}(c_{11} - c_{12})$  at  $T_N$ . On the other hand the shear constant  $c_{44}$  was found to vary smoothly through  $T_N$  showing no effects of magnetic origin.

The Cr + 2.6 at. % Al crystal was grown by a floating-zone method using RF heating. Parallel (110) faces were obtained by spark cutting. The diameter of the cylindrical

sample as well as the distance between the parallel (110) faces were both about 6 mm. Ultrasonic (10 Mhz) wave velocities were measured using a comparison method (Bohlmann and Alberts 1970) at temperature intervals of about 2 K from 77 to 400 K. In calculating the elastic constants from the wave velocities, we used a density value calculated from the lattice parameters (Chakrabarti and Beck 1971). Measurements of the longitudinal velocity along [110] gives the combination of elastic constants  $c_1 = \frac{1}{2}(c_{11} + c_{12} + 2c_{44})$  while shear velocity measurements give  $\frac{1}{2}(c_{11} - c_{12})$  and  $c_{44}$ . The experimental error in the absolute values of the wave velocities is estimated to be about 0.5%, while changes of the order of 1 in  $10^3$  with temperature could be detected.  $c_{11}$  and  $c_{12}$  were obtained from smooth curves drawn through the results for  $c_1$ ,  $\frac{1}{2}(c_{11} - c_{12})$  and  $c_{44}$ . In order to keep the crystal as large as possible for future neutron diffraction studies, no attempt was made to cut (100) faces on it for direct  $c_{11}$  measurements. No correction was made for the change of density and sample length with temperature as it follows from the thermal expansion measurements of Alberts and Lourens (1984) that these corrections are too small (of the order of  $10^{-3}$  at 77 K) to affect the qualitative features of the data significantly.

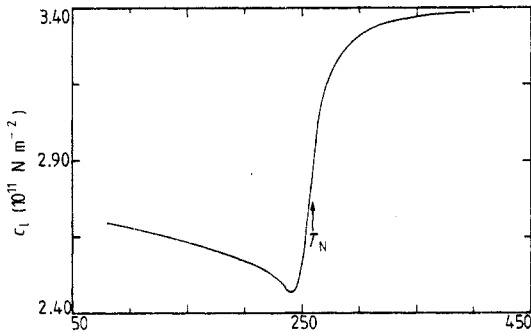
The concentration determined by electron microprobe analysing techniques was  $(2.6 \pm 0.2)$  at.% Al and the sample was found to be of good homogeneity. For this concentration the transition at  $T_N$  is a CSDW-P one (Alberts 1985).

The room-temperature (293 K) elastic constants of the single crystal of Cr + 2.6 at.% Al are found to be  $c_{11} = (3.60 \pm 0.05) \times 10^{11} \text{ N m}^{-2}$ ,  $c_{12} = (0.90 \pm 0.05) \times 10^{11} \text{ N m}^{-2}$  and  $c_{44} = (1.03 \pm 0.01) \times 10^{11} \text{ N m}^{-2}$ . For pure Cr,  $c_{11} = 3.552 \times 10^{11} \text{ N m}^{-2}$ ,  $c_{12} = 0.707 \times 10^{11} \text{ N m}^{-2}$  and  $c_{44} = 1.009 \times 10^{11} \text{ N m}^{-2}$  (van Rijn and Alberts 1983).

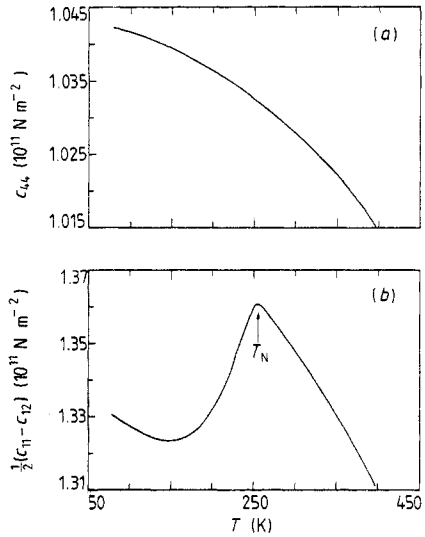
Figure 1 shows the temperature variation of  $c_1 = \frac{1}{2}(c_{11} + c_{12} + 2c_{44})$  and figure 2 that of  $c_{44}$  and  $\frac{1}{2}(c_{11} - c_{12})$ . The temperature dependence of  $c_{11}$ ,  $c_{12}$  and  $B = \frac{1}{3}(c_{11} + 2c_{12})$  is shown in figure 3.

In measuring  $c_1$  large ultrasonic attenuation was observed in a small temperature range just above the minimum in figure 1. The minimum at 238 K is fairly sharp while the attenuation reaches a maximum value around 255 K near the inflection point to the right of the minimum in figure 1. This temperature corresponds to within 5 K with the temperature where  $\frac{1}{2}(c_{11} - c_{12})$  in figure 2 reaches a maximum. Little change in attenuation was observed near 255 K in measuring the shear constant. The temperature of  $(255 \pm 5)$  K at the inflection point in figure 1 and at the peak in  $\frac{1}{2}(c_{11} - c_{12})$  was taken as  $T_N$  and also corresponds to the temperature at the inflection points to the right of the minima of  $c_{11}$ ,  $c_{12}$  and  $B$  (figure 3). For polycrystalline Cr-Al alloys  $T_N$  was defined in a similar manner (Alberts and Lourens 1984). The value  $T_N = (255 \pm 5)$  K of the Cr + 2.6 at.% Al single crystal corresponds well with the results of Alberts and Lourens (1984) on polycrystals.

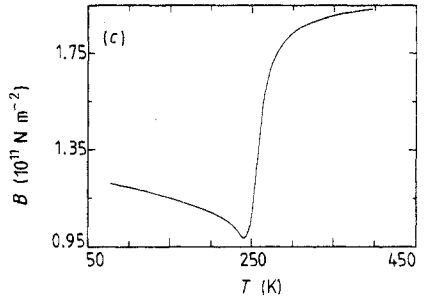
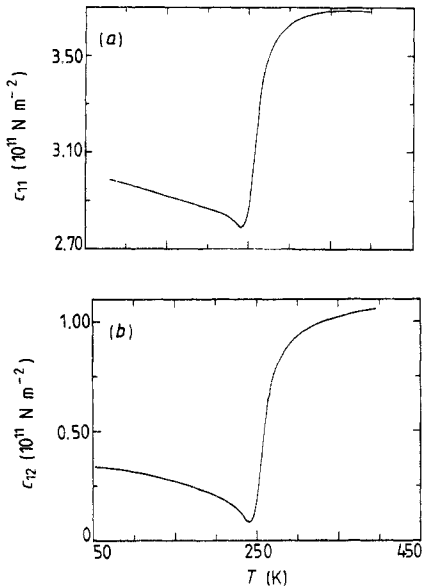
The main features of the behaviour of the elastic constants at the CSDW-P transition in Cr + 2.6 at.% Al compared to those of the ISDW-P transition in pure Cr are as follows. Firstly, the compressional constants  $c_1$ ,  $c_{11}$ ,  $c_{12}$  and the bulk modulus  $B$  of the former show a 'jump-like' transition at the CSDW-P transition where these quantities increase sharply to higher values in the paramagnetic region. In pure Cr, however, the ISDW-P transition is  $\lambda$ -type. Secondly, the shear constant  $\frac{1}{2}(c_{11} - c_{12})$  of Cr + 2.6 at.% Al shows a cusp at  $T_N$  with a minimum near 150 K, similar to pure Cr. The shear constant  $c_{44}$ , on the other hand, varies smoothly through  $T_N$  (figure 2) without any effects of magnetic origin while it shows a small anomaly in pure Cr near  $T_N$ . The increases in  $B$ ,  $c_{11}$  and  $c_{12}$  in going from the CSDW to the paramagnetic state of Cr + 2.6 at.% Al are approximately



**Figure 1.** Temperature dependence of the combination of elastic constants  $c_i = \frac{1}{2}(c_{11} + c_{12} + 2c_{44})$  of Cr + 2.6 at.% Al. The experimental error in the absolute values of  $c_i$  is about 1% while changes of the order of 1 in  $10^3$  with temperature could be detected. A smooth curve through the experimental points, which were taken at temperature intervals of about 2 K, is shown.  $T_N$  is the Néel temperature.



**Figure 2.** Temperature dependence of elastic constants (a)  $c_{44}$ , and (b)  $\frac{1}{2}(c_{11} - c_{12})$  of Cr + 2.6 at.% Al. Experimental errors and the smooth curve are explained in figure 1.



**Figure 3.** Temperature dependence of elastic constants (a)  $c_{11}$ , (b)  $c_{12}$  and bulk modulus (c)  $B = \frac{1}{3}(c_{11} + 2c_{12})$  of Cr + 2.6 at.% Al. The values were determined from the smooth curves of figures 1 and 2.

$0.9 \times 10^{11} \text{ N m}^{-2}$  for all three cases, which compare well with the polycrystalline bulk modulus values of Alberts and Lourens (1984). The anomaly in  $\frac{1}{2}(c_{11} - c_{12})$  is however much smaller, amounting to about  $0.04 \times 10^{11} \text{ N m}^{-2}$  between the minimum and maximum values of figure 2, which is about the same as for pure Cr.

No anomalies are observed in the shear constants of polycrystalline Cr-Al alloys (Alberts and Lourens 1984) and also not in other polycrystalline Cr alloys, except for the Cr-Si and Cr-Fe systems which show a first order change in thermal expansion at

$T_N$  (Alberts and Lourens 1988, Hausch and Török 1977). The fact that magnetic anomalies are not observed in the shear constants of polycrystalline material may be attributed to the relatively small value of the anomaly in  $\frac{1}{2}(c_{11} - c_{12})$  and its absence in  $c_{44}$ , resulting in a very small value of the anomaly in the shear constant when the single crystal elastic constants are averaged to obtain the polycrystalline value. For instance, using the Voigt average (Huntington 1958) to estimate the anomaly in the shear constant ( $G$ ) of polycrystalline Cr + 2.6 at.% Al, one obtains  $\Delta G = \frac{2}{15}\Delta(\frac{1}{2}(c_{11} - c_{12})) + \frac{1}{5}\Delta c_{44} \approx 0.005 \times 10^{11} \text{ N m}^{-2}$  using  $\Delta(\frac{1}{2}(c_{11} - c_{12})) \approx 0.04 \times 10^{11} \text{ N m}^{-2}$  and  $\Delta c_{44} = 0$  from our single-crystal measurements. This value of  $\Delta G$  is about 200 times smaller than that of  $\Delta B$  and difficult to observe experimentally, as coupling shear waves to the sample is usually much more difficult than for compressional waves.

We conclude that the CSDW-P transition in a single crystal of Cr + 2.6 at.% Al is characterised by a jump-like transition in the single-crystal compressional constants and by a cusp-like anomaly in the shear constant  $\frac{1}{2}(c_{11} - c_{12})$ . No anomaly was observed in the shear constant  $c_{44}$ . Except for  $\frac{1}{2}(c_{11} - c_{12})$  the behaviour of the other elastic constants differs from those observed at the ISDW-P transition of pure Cr.

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