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LETTER TO THE EDITOR

Elastic constants of a single crystal of Cr + 5 at.% V

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Abstract. The elastic constants of a single crystal of Cr + 5 at.% V were measured in the temperature range 77-480 K. The results can be used as representative of the non-magnetic behaviour in determining the magnetic contributions to the single-crystal elastic constants of Cr and its dilute alloys. Using the results on the Cr + 5 at.% V single crystal it is shown that there is a change of sign in the magnetic contributions to c_{44} and $\frac{1}{2}(c_{11} - c_{12})$ of pure Cr below the spin-flip transition temperature.

Cr and its alloys are spin density wave antiferromagnetic materials, of which the magnetoelastic properties have received much attention during the last decade (Fawcett and Alberts 1990). Of particular importance are the magnetic contributions to the thermal expansion and elastic constants of these materials. In determining these contributions it is necessary to compare the measured quantities with a suitable nonmagnetic system of similar lattice dynamics. As the addition of more than 4 at.% V to Cr destroys antiferromagnetism at all temperatures without changing the lattice parameter and density by more than one to two parts in a thousand, Roberts *et al* (1983) used the temperature behaviour of the thermal expansion coefficient, $\alpha(T)$, of polycrystalline Cr + 5 at.% V as representative of the non-magnetic behaviour of Cr. This was also done by Alberts and Lourens (1988) in determining the magnetovolume of several polycrystalline dilute Cr alloys. Concerning the bulk modulus of polycrystalline Cr alloys, Alberts and Lourens (1988) also used the elasticity of polycrystalline Cr + 5 at.% V for the non-magnetic behaviour.

Currently no successful theory exists (Alberts and Lourens 1988) for predicting the temperature behaviour of the elasticity of Cr and its alloys. For testing any future theory accurately, results for the single-crystal elastic constants of these materials are needed, and especially the magnetic contribution to these constants. Recently single-crystalline elastic constants of dilute Cr alloys have started to appear in the literature (Alberts 1989, de Camargo and Brotzen 1982). In order to obtain magnetic contributions to the single-crystal elastic constants $c_{11}, \frac{1}{2}(c_{11} - c_{12})$ and c_{44} , the nonmagnetic behaviour of these modes is required. Although $c_{11}, \frac{1}{2}(c_{11} - c_{12})$ and c_{44} were previously measured (de Camargo and Brotzen 1982) on Cr + 0.67 at.% V and on Cr + 1.5 at.% V, which both show antiferromagnetic behaviour below $T_{\rm N} = 244$ K and 174 K, respectively, no work was done on single crystals of Cr + 5 at.% V that can be used for the non-magnetic behaviour in determining the magnetic contributions to $c_{11}, \frac{1}{2}(c_{11} - c_{12})$ and c_{44} for Cr and its dilute alloys. We report here the temperature dependence of the elastic constants of a Cr + 5 at.% V single crystal.

The single crystal was grown by a floating-zone method, using RF heating, from 99.996 % pure Iochrome (Materials Research Corporation, New York) and Specpure V (Johnson-Matthey, UK). Parallel (110) faces were obtained by spark cutting. The diameter of the near 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 phase comparison method (Bohlmann and Alberts 1970) at temperature intervals of 2 K from 77-480 K for longitudinal waves and from 77-430 K for shear waves. The upper temperature limits were set by the transducer bonding agent (Araldite epoxy resin). Measurement of the longitudinal wave 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 the bulk modulus $B = \frac{1}{3}(c_{11} + 2c_{12})$ were obtained from smooth curves drawn through the results for $c_1, \frac{1}{2}(c_{11}-c_{12})$ and c_{44} . No corrections were made for the changes of density and sample length with temperature, because they follow from the thermal expansion measurements of Roberts et al (1983) that these corrections are too small (smaller than 0.1% at 77 K) to affect the data significantly.



Figure 1. Elastic constants $c_{11}, c_{44}, \frac{1}{2}(c_{11} - c_{12})$ and B of Cr + 5 at.% V as a function of temperature. The full curves are drawn through the experimental points, which were measured at 2 K intervals. The broken curves are back extrapolations from 77 K. The experimental error in the absolute values of the elastic constants amounts to about 1% while changes with temperature of 1 in 10^3 could be detected.

Table 1. Experimental values of the elastic constants of Cr + 5 at.% V in units of 10^{11} N m⁻² at 10 K intervals. Values below 77 K and above 480 K were obtained by extrapolation.

<i>T</i> (K)	c ₁₁	$\frac{1}{2}(c_{11}-c_{12})$	C44	$B = \frac{1}{3}(c_{11} + 2c_{12})$
0	4.011	1.469	0.998	2.052
10	4.009	1.468	0.998	2.052
20	4.009	1.468	0.998	2.052
30	4.007	1.467	0.998	2.051
40	4.005	1.466	0.998	2.050
50	4.005	1.466	0.997	2.050
60	4.003	1.465	0.997	2.050
70	4.000	1.463	0.997	2.049
80	3.998	1.462	0.996	2.049
90	3.996	1.461	0.996	2.048
100	3.993	1.459	0.995	2.048
110	3.990	1.457	0.994	2.047
120	3.986	1.455	0.994	2.046
130	3.984	1.454	0.993	2.045
140	3.979	1.452	0.993	2.043
150	3.975	1.449	0.992	2.043
160	3.971	1.447	0.991	2.042
170	3.966	1.444	0.991	2.041
180	3.961	1.442	0.990	2.038
190	3.957	1.439	0.989	2.038
200	3.951	1.436	0.988	2.036
210	3.946	1.433	0.987	2.035
220	3.941	1,430	0.986	2.034
230	3.934	1.427	0.986	2.031
240	3.929	1.424	0.985	2.030
250	3.923	1.421	0.984	2.028
260	3.917	1.418	0.983	2.026
270	3.912	1.415	0.982	2.025
280	3.906	1.412	0.981	2.023
290	3.900	1.408	0.980	2.023
300	3.894	1.405	0.979	2.021
310	3.888	1.402	0.978	2.019
320	3.883	1.399	0.977	2.018
330	3.876	1.395	0.976	2.016
340	3.870	1.392	0.975	2.014
350	3.865	1.389	0.974	2.013
360	3.857	1.385	0.973	2.010
370	3.851	1.382	0.972	2.008
380	3.845	1.379	0.971	2.006
390	3.838	1.375	0.970	2.005
400	3.832	1.372	0.969	2.003
410	3.827	1.369	0.967	2.002
420	3.820	1.365	0.966	2.000
430	3.814	1.362	0.965	1.998
440	3.807	1.358	0.964	1.996
450	3.801	1.355	0.963	1.994
460	3.796	1.352	0.961	1.993
470	3.789	1.348	0.960	1.992
480	3.783	1.345	0.959	1.990
490	3.777	1.342	0.958	1.988
500	3.771	1.338	0.956	1.987



Figure 2. The elastic constants (Katahara *et al* 1979) of pure Cr (full curves) compared with the non-magnetic behaviour (broken curves) as obtained from the measurements on Cr + 5 at % V.

The single-crystal elastic constants of Cr + 5 at.% V at room temperature are

$$\frac{1}{2}(c_{11} - c_{12}) = (1.410 \pm 0.005) \times 10^{11} \text{ N m}^{-2}$$

$$c_{11} = (3.90 \pm 0.03) \times 10^{11} \text{ N m}^{-2}$$

$$\frac{1}{2}(c_{11} - c_{12}) = (1.408 \pm 0.005) \times 10^{11} \text{ N m}^{-2}$$

$$c_{44} = (0.980 \pm 0.007) \times 10^{11} \text{ N m}^{-2}.$$

For pure Cr the constants at room temperature are (van Rijn and Alberts 1983)

$$\frac{1}{2}(c_{11} - c_{12}) = 1.423 \times 10^{11} \text{ N m}^{-2}$$

$$c_{11} = 3.55 \times 10^{11} \text{ N m}^{-2}$$

$$\frac{1}{2}(c_{11} - c_{12}) = 1.42 \times 10^{11} \text{ N m}^{-2}$$

$$c_{44} = 1.01 \times 10^{11} \text{ N m}^{-2}.$$

Figure 1 shows the variation of $c_{11}, c_{44}, \frac{1}{2}(c_{11}-c_{12})$ and B with temperature while values at 10 K intervals are given in table 1. Although measurements were carried out in the temperature range 77-480 K for longitudinal modes and 77-430 K for the shear modes, the near-linear behaviour above 300 K allows for accurate extrapolation in obtaining $c_{11}, c_{44}, \frac{1}{2}(c_{11}-c_{12})$ and B up to 500 K. The values in the temperature range 0-77 K were obtained by back extrapolation, which could be done to better than about 0.3% of the absolute value at 0 K for c_1 , 0.5% for $\frac{1}{2}(c_{11}-c_{12})$ and 0.1% for c_{44} . This is reasonable when compared with the total changes of about 5% for c_1 , 10% for $\frac{1}{2}(c_{11}-c_{12})$ and 4% for c_{44} over the total temperature range.

The temperature dependence of the elastic constants of Cr was measured by several authors (Palmer and Lee (1971), Bolef and de Klerk (1963), van Rijn and Alberts (1983), Katahara *et al* (1979) and Muir *et al* (1987)). Magnetic effects were found to exist in some of the constants up to about 500 K. Only the work of Katahara *et al* (1979) was done to high enough temperatures (up to 700 K) to enable back extrapolation, using the measurements on the Cr + 5 at.% V single crystal, to obtain the magnetic contributions. The back extrapolation is shown in figure 2. Here the curves for Cr + 5 at.% V were translated slightly up or down to coincide with the high-temperature behaviour of pure Cr.

The magnetic contribution to c_{11} , $\Delta c_{11} = c_{11}$ (non-magnetic) $-c_{11}$ (antiferromagnetic), decreases from 0.17×10^{11} N m⁻² to 0.03×10^{11} N m⁻² in going from just above the spin-flip transition temperature, $T_{\rm SF} = 123$ K, down to 77 K. Δc_{11} is positive at all temperatures and disappears at about 500 K (figure 2). In the case of c_{44} the magnetic contribution $\Delta c_{44} = c_{44}$ (non-magnetic) $-c_{44}$ (antiferromagnetic) disappears just above the Néel temperature $(T_{\rm N})$. It is positive for $T_{\rm N} > T > T_{\rm SF}$ and changes sign to negative values for T just below $T_{\rm SF}$. The situation is the same for $\frac{1}{2}(c_{11}-c_{12})$. The change in sign of Δc_{44} and $\Delta \frac{1}{2}(c_{11}-c_{12})$ below $T_{\rm SF}$ is a new effect that could not previously be observed due to the lack of accurate data for the non-magnetic state.

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