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The Anisotropy of the Thermal Expansion of α-Titanium

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In order to resolve the discrepancy found in earlier work, the anisotropic thermal expansion of α-titanium has been determined by the X-ray method. If a small range of temperature is used the coefficient of expansion observed along the hexagonal axis (α_c) is smaller than that in the basal plane (α_a). The nature of the deviation of the α-titanium structure from ideal hexagonal close-packing and the room temperature elastic behaviour of the metal have been shown to be in agreement with the result that α_c ($5{\cdot}6\times10^{-6}.°C^{-1}$) is smaller than α_a ($9{\cdot}5\times10^{-6}.°C^{-1}$).

As the room temperature value of the axial ratio of α-titanium (1·588) is smaller than that for an ideal close-packed hexagonal structure (1·633), the immediate neighbours of any atom lying in the basal plane are at distances larger than those at which immediate neighbours from the adjacent planes are situated. This deviation from the ideal structure can be said to be a consequence of stronger interatomic bonding along the hexagonal axis than that in the basal planes and hence, in a general way, it may be expected that the coefficient of thermal expansion parallel to the *c* axis (α_c) will be smaller than that along the *a* axis (α_a) (Childs, 1953). However, the experimental data on the thermal expansion of this metal, available from published literature, are found to be conflicting. While Berry & Raynor (1953) and Spreadborough & Christian (1959) have reported that α_c is greater than α_a, Brocklehurst (1953) gives just the opposite result. (See Table 2 of this paper.) Besides, there are well established observations that the *c* parameter of α-titanium is very sensitive to contamination of the metal by oxygen and nitrogen. This effect has been reported to be very prominent at high temperatures (Clark, 1949; Spreadborough & Christian, 1959), of the order of 600°C, and has been observed even if the metal is sealed in (conventionally) evacuated tubes (Berry & Raynor, 1953). To solve this problem and to find the real nature of the anisotropy of the thermal expansion of α-Ti, the authors undertook a redetermination of its lattice parameters, at different temperatures, over a range within which the possibility of the air-contamination is negligible. The results reported below show that if the heating of the sample is limited to a small range of temperature, the coefficient of expansion α_c is smaller than the coefficient α_a, a result in agreement with Brocklehurst's data.

The X-ray diffraction work was done on a 19 cm diameter high temperature camera. The method of using this camera has been described earlier (Deshpande & Pawar, 1962). 'Specpure' α-titanium was used in preparing the specimen. Reflexions from six planes, recorded in the high angle region between $\theta=60°$ and $\theta=80°$ were measured and used in the evaluation of the lattice parameters. Pictures were taken at four different temperatures between 28 and 155°C. No attempt was made to go to high temperatures, because of the fear of contamination of the powder specimen by atmospheric oxygen and nitrogen. A room temperature picture, taken after the specimen was cooled, showed that no contamination had taken place as a result of the heating involved during the exposure (Table 1). Each film was measured repeatedly and the readings were processed by Cohen's method of least squares to give the value of the lattice constants.

Table 1. *Values of the lattice parameters and axial ratio of α-titanium at different temperatures*

Temperature	*a*	*c*	*c*/*a*
28°C	2·9508 ± 0·0002 Å	4·6855 ± 0·0003 Å	1·5880
65	2·9524	4·6871	1·5875
100	2·9531	4·6875	1·5873
155	2·9543	4·6892	1·5872
28	2·9505	4·6855	1·5880

Table 2. *Comparison of the results of different investigators on the thermal expansion of α-titanium*

Author	$\alpha_a\times10^6$ ($°C^{-1}$)	$\alpha_c\times10^6$ ($°C^{-1}$)	$\alpha_{av}\times10^6$ ($°C^{-1}$)	Temperature range (°C)
Erfling (1942)	–	–	8·24	20–40
Greiner & Ellis (1949)	–	–	9·0	30–200
Brocklehurst (1953)	11·0	8·8	10·3	25–225
Berry & Raynor (1953)	11·03	13·37	11·81	r.t.–700
Spreadborough & Christian (1959)	9·55	10·65	9·92	0–600
Present work	9·5	5·6	8·2	28–155

Table 1 gives the values of the lattice constants of α-titanium at different temperatures, along with the values of the axial ratio and the standard errors in the values of the parameters calculated, for the film at room temperature, by the method of Jette & Foote (1935). Both the parameters were found to vary linearly with temperature, within the limits of the experimental errors. From the gradients of the temperature *versus* parameters graphs, the two principal coefficients of expansion were calculated. The values are found to be

$$\alpha_c = 5{\cdot}6 \times 10^{-6}.°C^{-1}$$
$$\alpha_a = 9{\cdot}5 \times 10^{-6}.°C^{-1}.$$

Table 2 gives a summary of the results on the coefficients of thermal expansion obtained by different workers, with the respective ranges of temperature used. As already mentioned, the nature of the anisotropy of thermal expansion reported by Brocklehurst (1953) is opposite to that found by Berry & Raynor (1953) and Spreadborough & Christian (1959). The present results are in agreement with those of Brocklehurst and satisfy the expectation regarding the type of anisotropy for a metal with axial ratio smaller than the value for ideal close-packed structure. An interesting point to be noted, in this respect is that, whereas both Brocklehurst and the present authors have worked in a small range from room temperature to about 200 °C, neither Berry & Raynor (1953) nor Spreadborough & Christian (1959) have made any measurement in this range. It is also interesting to note that the values of the average coefficient of thermal expansion reported by Erfling (1942) and Greiner & Ellis (1949) are in good agreement with the corresponding value obtained from the present results and that these investigators have worked at temperatures below 200 °C. Yet another point in support of the present results comes from the calculation of the linear compressibilities of the metal along the *a* and *c* axes, from the single-crystal elastic constants reported by Flowers, O'Brien & McEleney (1964). Following the method given by Boas & Mackenzie (1950), the values of the linear compressibilities come out as

$K_c = 3{\cdot}019 \times 10^{-13}$ cm².dyne^{-1} (along the *c* axis)
$K_a = 3{\cdot}314 \times 10^{-13}$ cm².dyne^{-1} (along the *a* axis).

These results show that the binding between the neighbouring atoms in the basal plane is weaker than that between atoms in the adjacent planes and so the atomic displacements, whether due to hydrostatic pressure or to an increase in temperature, will be easier and larger along the *a* axis than those along the *c* axis.

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