

to 1000 °C. TiC is face-centred cubic with $a=4.32$ Å, and rutile is body-centred tetragonal with $a=4.59$, $c=2.96$ Å. The present note reports the identification of the orientation relationship between the oxide film and the parent carbide crystal.

The orientation of a flake of rutile which had been cleaved from the TiC crystal was determined by taking a series of X-ray oscillation photographs. From these photographs it was evident that the oxide grows with

its (110) plane parallel to the (100) TiC surface. Each photograph showed reflections from two (110) rutile films which are orthogonally inclined about the [110] axis.

To find the complete orientation relationship, a TiC crystal having its oxide surface layer intact was examined by taking glancing-incidence oscillation photographs, the axis of oscillation being parallel to a cube axis. It was found that the rutile tetrad axis is parallel to one of the TiC cube axes lying in the surface of the crystal so that the complete orientation relationship is

$$(100) \text{TiC} \parallel (110) \text{TiO}_2 \text{ with } [010] \text{TiC} \parallel [001] \text{TiO}_2.$$

As before, two strong rutile patterns were obtained simultaneously, corresponding to the two possible orientations of the tetrad axis given above.

Comparison of the lattice vectors (x) which define the above orientation relationship shows that

$$x[010]\text{TiC}/x[001]\text{TiO}_2 = 1.46 \text{ and} \\ x[001]\text{TiC}/x[\bar{1}10]\text{TiO}_2 = 0.667$$

which means that, at the carbide-oxide interface, three $x[010]\text{TiC}$ vectors fit two $x[001]\text{TiO}_2$ vectors with a misfit of only 2.74% and that two $x[001]\text{TiC}$ vectors match three $x[\bar{1}10]\text{TiO}_2$ vectors with no misfit. Consequently, we postulate an oxidation mechanism based on the re-arrangements of titanium atoms shown in Fig. 1. This involves only small lateral translations. During oxidation there is no requirement for titanium atoms to diffuse outwards normally to the parent TiC (100) surface but as each successive sheet of Ti atoms reacts there must be an overall uniform movement of the rutile film along the [100] TiC direction to allow for the difference in specific volume.

We are indebted to the Director of Berkeley Nuclear Laboratories for permission to publish this work.

Reference

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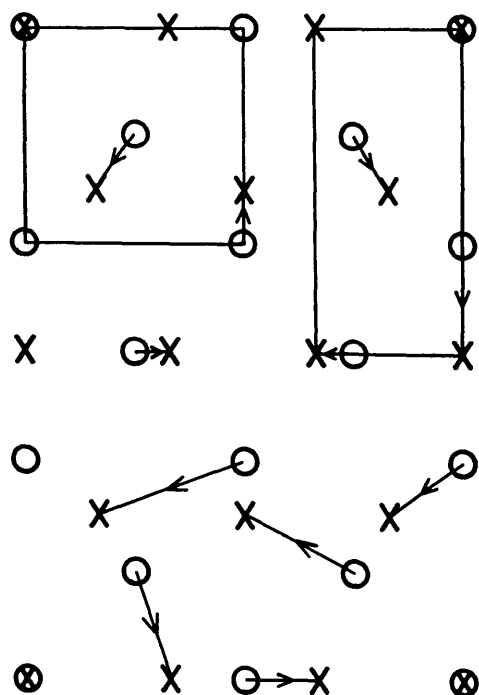


Fig. 1. Titanium atomic positions at the carbide-oxide interface. Positions in TiC are denoted \circ , positions in TiO_2 \times . The arrows indicate one possible set of small lateral movements of Ti atoms which would be involved in the oxidation of this plane of TiC to TiO_2 .

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The unit-cell dimensions of silver azide. By H. E. MARR, III and R. H. STANFORD, JR., *Gates and Crellin Laboratories of Chemistry,* California Institute of Technology, Pasadena, California, U. S. A.*

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Crystallographic studies of silver azide, AgN_3 , have been made by Bassiere (1935), West (1936), Hughes (1935), Pfeiffer (1949), and Dewing, Hughes, & Pfeiffer (1962). It crystallizes in the orthorhombic space group *Ibam* and the unit cell dimensions given by previous investigators are:

	a_0	b_0	c_0
Bassiere	5.59 Å	5.94 Å	6.05 Å
West	5.59	5.91	5.97
Hughes	5.66	5.94	5.99
Dewing <i>et al.</i>	5.60	5.92	6.00

* Contribution No. 2870 from the Gates and Crellin Laboratories of Chemistry.

The structure has been accurately determined (Dewing, Hughes, & Pfeiffer, 1962); but accurate cell dimensions and, hence, accurate bond lengths have been lacking. The determination of these dimensions was undertaken as an undergraduate research project.

The powder sample was prepared by mixing equimolar solutions of silver nitrate and sodium azide and allowing the precipitate to form in the dark over night. Two powder photographs were taken with a Straumanis-type camera with a nominal radius of 9.9662 cm. using $\text{Cu } K\alpha$ radiation. Potassium chloride lines were superimposed on one of the photographs to provide a check.

The α_1 and α_2 doublets of three high angle reflections which could be unambiguously indexed were measured

and these data were used to determine the lattice constants by least squares. The procedure minimized the function

$$\varphi = \sum w_i \{(\sin^2 \theta_c)_i - (\sin^2 \theta_0)_i\}$$

where the weights, w , were taken proportional to $1/\sin^2 2\theta$.

The values of the unit cell dimensions and their standard deviations obtained from this least squares procedure are:

$$a_0 = 5.6170 \pm 0.0005, \quad b_0 = 5.9146 \pm 0.0003, \\ c_0 = 6.0057 \pm 0.0005 \text{ \AA}.$$

The value of a_0 for potassium chloride was found to be $6.2933 \pm 0.0009 \text{ \AA}$, which may be compared with the

value 6.29294 \AA which was determined by Hambling (1953). The wavelengths for Cu K radiation were assumed to be those given by Bragg (1947)

$$\alpha_1: 1.54050, \quad \alpha_2: 1.54434 \text{ \AA}.$$

Table 1 shows the observed and calculated values of $\sin \theta$ for the reflections used.

The density as measured by previous investigators is:

Bassiere	4.81 g.cm. ⁻³
West	4.50
Hughes	4.837

Hughes has indicated that his procedure probably leads to a low result, so that his value should represent the lower limit. The calculated value for the density, using the cell dimensions of this investigation, is 4.99 g.cm.^{-3} .

Table 1. Observed and calculated values of $\sin \theta$

hkl	Film 1	Film 2	$\sin \theta_c$
AgN_3	$\sin \theta_0$	$\sin \theta_0$	
462 α_2	0.99108	0.99103	0.99100
462 α_1	0.98847	0.98849	0.98854
426 α_2	0.98265	0.98268	0.98268
426 α_1	0.98027	0.98023	0.98023
604 α_2	0.97183	0.97180	0.97202
604 α_1	0.96983	0.96979	0.96961
KCl			
800 α_2	0.98173		0.98188
800 α_1	0.97964		0.97947
642 α_2	0.91941		0.91939
642 α_1	0.91710		0.91713

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Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the General Secretary of the International Union of Crystallography (D. W. Smits, Mathematisch Instituut, University of Groningen, Reithdiepskade 4, Groningen, The Netherlands).

Appointment of Technical Editor

As already announced in this journal, the Executive Committee of the Union decided at its meeting in Munich that the time had come to appoint a full-time technical editor for the publications of the Union; and applications for this post were invited soon thereafter. The matter had become urgent because the increasing size of *Acta Crystallographica* had made it impossible to find a successor to Prof. Asmussen, who had requested to be relieved of the technical editorship of the journal with the completion of the 1962 volume.

The Executive Committee is glad to announce the appointment of Mr S. A. Bryant to the new post. Mr Bryant studied chemistry and crystallography in Oxford, where he obtained his B. A. with First Class Honours and the research degree of B.Sc. After a two-year lectureship at Armstrong (now King's) College, Newcastle, and another two-year period of structure research at

Bristol University, he joined the Department of Scientific and Industrial Research as a Scientific Officer at the Forest Products Research Laboratory at Princes Risborough. Ten years later he became attached to Shell, originally as research chemist, but some three years later he was charged with the supervision and reorganization of a large library and a documentation and technical enquiry service which served as a central technical information organization for the world-wide Shell Group. Since 1952 Mr Bryant had been working as Senior Technical Editor at the Shell Thornton Research Centre.

Mr Bryant started his work for the Union on 15 November 1962. It is the intention that as soon as he has become acquainted with the technical editorship of *Acta Crystallographica*, he will also devote himself to the technical side of the editing of *Structure Reports*, and gradually of the other publications of the Union. His office address is 9 Queensway, Newton Lane, Chester, England.