

Synthesis of a high-density phase of silicon dioxide in shock waves

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The crystal structure of silicon dioxide compressed by finite-amplitude shock waves of 350, 500, 700 and 900 kbar was investigated by x-ray structure analysis. Shock waves of 700 and 900 kbar amplitude transformed the α quartz lattice of silicon dioxide into an orthorhombic lattice with the parameters $a = 4.30 \text{ \AA}$, $b = 4.70 \text{ \AA}$, and $c = 4.50 \text{ \AA}$. The crystal density of the new phase of silicon dioxide calculated on basis of the lattice parameters is $\rho = 4.435 \text{ g/cm}^3$.

We investigated the crystal structure of silicon dioxide samples subjected to momentary loading with a series of shock waves of 350, 500, 700 and 900 kbar final amplitude. The loading of the samples and their subsequent storage was carried out in special bomb apparatus of the sort described in^[1]. The test samples were cut into disks 16 mm diam and 1 mm thick out of natural quartzite and single-crystal α -quartz. In both cases the initial density was $\rho = 2.65 \text{ g/cm}^3$. The crystal structure of the compressed samples was studied with an URS-50 x-ray diffractometer. The readings were taken from the flat surface of the crystals. An x-ray tube with bronze anticathode in conjunction with a nickel filter was employed as the radiation source.

Compression of the samples to $P = 350 \text{ kbar}$ left the diffraction picture relatively unchanged: the diffraction patterns showed some intensification of the diffuse background along with the α -quartz lines. Crystals subjected to pressures of up to 500 kbar were characterized by the absence of diffraction maxima and a very strong diffuse background (especially in the small-angle region). Analogous results had been obtained previously by Wackerly^[2] with quartz compressed by shock waves of amplitude 250 to 500 kbar.

Samples compressed at 700 and 900 kbar gave diffraction patterns with a number of diffraction maxima along with the background. The observed interplanar distances d_{obs} , calculated from the positions of the maxima on the diffraction patterns, are listed in the table below. It should be mentioned that all diffraction maxima were strongly broadened, but the maxima corresponding to reflection from faces with high values of hkl (Miller indices) were at the background level. This is most probably due to the stressed condition of the substance after shockloading. Furthermore, the presence of a rather marked diffuse background suggests that only a small portion of the substance is in the crystalline state, while the greater portion is possibly in the form of the so-called "shortrange"-order phase with sixfold coordination of its nearest neighbors^[3].

The indexing of the diffraction patterns was achieved by using as a basis an orthorhombic lattice similar to that described in^[4], where a new crystalline modifica-

| d_{obs} | Intensity | hkl | d_{calc} | d_{obs} | Intensity | hkl | d_{calc} |
|------------------|-----------|-------|-------------------|------------------|-----------|-------|-------------------|
| 3.15 | weak | 110 | 3.175 | -- | — | 022 | 1.626 |
| 2.59 | strong | 111 | 2.594 | 1.58 | weak | 220 | 1.588 |
| 2.35 | moderate | 020 | 2.351 | 1.55 | weak | 202 | 1.555 |
| 2.25 | moderate | 002 | 2.250 | -- | — | 122 | 1.521 |
| 2.15 | moderate | 200 | 2.152 | 1.49 | moderate | 221 | 1.497 |
| 2.08 | strong | 021 | 2.084 | 1.35 | very weak | 113 | 1.357 |
| 1.99 | weak | 102 | 1.994 | 1.31 | very weak | 311 | 1.312 |
| 1.88 | very weak | 121 | 1.875 | -- | — | 222 | 1.297 |
| -- | — | 112 | 1.836 | 1.24 | very weak | 132 | 1.232 |

tion of TiO_2 having an orthorhombic lattice with space group Pbcn and four TiO_2 molecules per unit cell was synthesized under static conditions. The new quartz phase has parameters $a = 4.30 \text{ \AA}$, $b = 4.70 \text{ \AA}$, and $c = 4.50 \text{ \AA}$. The interplanar distances d_{cal} calculated with the above parameters (see the table) agree satisfactorily with the observed values d_{obs} .

No detailed calculation was made of the line intensities of new SiO_2 phase, but a comparison of the relative magnitude of the diffraction maxima on the patterns with the relative intensities of new TiO_2 phase gives satisfactory agreement. The crystal density calculated from the lattice parameters is $\rho = 4.435 \text{ g/cm}^3$. It is pointed out that, owing to the rather strong broadening of the diffraction maxima and also the absence of maxima at high hkl values, the lattice parameters could not be determined to a precision greater than $\pm 0.01 \text{ \AA}$.

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¹I. N. Dulin, L. V. Al'tschuler, V. Ya. Vashchenko, and V. N. Zubarev, Fiz. Tverd. Tela 11, 1252 (1969) [Sov. Phys.-Solid State 11, 1016 (1969)].

²J. Wackerly, J. Appl. Phys. 33, 922 (1962).

³P. S. De Carli, and D. J. Milton, Science 147, 144 (1965).

⁴N. A. Bendeliani, C. V. Popova, and L. F. Vereshchagin, Geokhimia 5, 499 (1966).

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