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X-ray determination of thermal expansion of zinc oxide. By AIJAZ A. KHAN, *Regional Research Laboratory, Hyderabad, India*

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Lattice parameters of zinc oxide have been determined accurately at different temperatures between 27 °C and 619 °C. These data have been processed to evaluate the temperature variation of the coefficients of thermal expansion α_a and α_c and the results could be represented as follows:

$$\alpha_a = 6{\cdot}05 \times 10^{-6} + 2{\cdot}20 \times 10^{-9}t + 2{\cdot}29 \times 10^{-12}t^2\,°C^{-1}$$
$$\alpha_c = 3{\cdot}53 \times 10^{-6} + 2{\cdot}38 \times 10^{-9}t + 9{\cdot}24 \times 10^{-14}t^2\,°C^{-1}$$

where t is the temperature in °C.

Lattice parameters of zinc oxide have been determined at room temperature by several workers (Bunn, 1935; Heller, McGannon & Weber, 1950; Rymer & Archard, 1952; Mohanty & Azaroff, 1961; Sirdeshmuk, 1963; Khan, 1966). Among these, only Sirdeshmuk (1963) has determined the lattice parameters in the high-temperature region also, at 196 °C and 267 °C and calculated the coefficients of thermal expansion from his results. This note gives the results of a systematic study, made in this Laboratory, on the temperature variation of the lattice parameters and the coefficients of expansion of zinc oxide, in the range 27–619 °C.

A 19·0 cm diameter high-temperature Unicam powder camera, calibrated with silver for high-temperature investigations, was employed along with Ni-filtered copper radiation. Fluctuations in specimen temperature were minimized by supplying power through a voltage stabilizer. Extra pure grade zinc oxide, supplied by E. Merck, was used for taking powder patterns at fourteen different temperatures between 27°C and 619°C. Several $\alpha_1\alpha_2$ doublets, with measurable intensities, were recorded in the high-angle region and, depending upon the quality of films, between nine and thirteen of these lines were carefully measured. Lattice parameters and their standard errors were calculated using an IBM 1620 computer. The program of calculations involved Cohen's (1935) analytical method with Nelson & Riley's (1945) extrapolation function for the evaluation of lattice parameters, and Jette & Foote's (1935) method for estimating the standard errors.

Table 1 gives the values of the a and c parameters at different temperatures along with their errors. Graphs of lattice parameter against temperature indicated that both the parameters changed non-linearly with temperature. Coefficients of expansion were calculated from the graphs at small and regular intervals of temperature and a statistical adjustment of these data gave the following equations for the two coefficients, α_a and α_c:

$$\alpha_a = 6{\cdot}05 \times 10^{-6} + 2{\cdot}20 \times 10^{-9}t + 2{\cdot}29 \times 10^{-12}t^2\,°C^{-1}$$
$$\alpha_c = 3{\cdot}53 \times 10^{-6} + 2{\cdot}38 \times 10^{-9}t + 9{\cdot}24 \times 10^{-14}t^2\,°C^{-1},$$

where t is the temperature in °C. The values of α_a and α_c at 25 °C, obtained from slight extrapolations of the present results are $6{\cdot}11 \times 10^{-6}.°C^{-1}$ and $3{\cdot}59 \times 10^{-6}.°C^{-1}$, respectively. The values obtained near room temperature by Sirdeshmuk (1963) as $\alpha_a = 6{\cdot}49 \times 10^{-6}.°C^{-1}$ and $\alpha_c = 3{\cdot}24 \times 10^{-6}.°C^{-1}$, agree well with the present values.

Table 1. *Lattice parameters of zinc oxide at different temperatures*

Temperature	a	c
27 °C	3·2500 ± 0·0001 Å	5·2070 ± 0·0004 Å
128	3·2522 ± 0·0002	5·2098 ± 0·0007
225	3·2540 ± 0·0001	5·2108 ± 0·0005
250	3·2548 ± 0·0001	5·2109 ± 0·0005
288	3·2553 ± 0·0001	5·2121 ± 0·0005
339	3·2566 ± 0·0001	5·2130 ± 0·0004
349	3·2569 ± 0·0001	5·2141 ± 0·0004
420	3·2588 ± 0·0001	5·2164 ± 0·0006
453	3·2591 ± 0·0001	5·2154 ± 0·0006
504	3·2606 ± 0·0001	5·2167 ± 0·0004
515	3·2612 ± 0·0002	5·2185 ± 0·0006
543	3·2616 ± 0·0001	5·2178 ± 0·0004
563	3·2620 ± 0·0001	5·2183 ± 0·0004
619	3·2637 ± 0·0001	5·2204 ± 0·0006

An interesting observation has been made by Archard (1953) about the value of c/a for zinc oxide subjected to different atmospheric conditions; it decreased slightly (1 part in 5000), if the sample was exposed to the ordinary atmosphere instead of dry air or dry oxygen and nitrogen. To explain his results he assumed a lattice distortion, occurring owing to some atmospheric contamination, involving a change of crystal symmetry. However, there appears to be no subsequent report confirming this observation and in the present work also no attempt has been made to study the probable change of symmetry. In any case, the assumption of a hexagonal unit cell will be true within the limits of estimated errors.

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