Acta Cryst. (1966). **21**, 290

Coefficient of expansion of gallium arsenide from -62 to 200°C.

By E. D. PIERRON, D. L. PARKER and J. B. MCNEELY, *Monsanto Central Research Laboratory, St. Louis, Mo., U.S.A.*

(*Received* 13 *January* 1966)

Recently Straumanis & Kim (1965) and Shaw Nan & Liu Yi-Huan (1965) reported precise lattice constants of gallium arsenide at temperature ranges from 5 to 65°C and from 23 to 735°C respectively.

The purpose of this study was to confirm the expansion coefficient values and to extend the range investigated especially toward the lower temperature, −62°C.

The gallium arsenide sample used was synthesized from Alcoa 99·9999 % gallium and Cominco 99·9999 % arsenic. The impurity level in the synthesized GaAs was less than 1·0 ppm as determined by emission spectrography and confirmed by Hall effect and electron mobility measurements.

The sample was ground to pass a No. 325 sieve (44 microns) and annealed at 400°C overnight to relieve the internal stresses introduced in the grinding operation.

The X-ray powder patterns were obtained with Cu radiation on a General Electric XRD-5 diffractometer which was equipped with a Materials Research Corporation high temperature X-ray diffractometer attachment Model X-86G. This attachment permits mounting the sample vertically in a parafocusing geometry. The temperatures were measured by means of calibrated thermocouples: copper–constantan for temperatures lower than 24°C and platinum–platinum-13 % rhodium for 24°C and higher. It was ascertained that the temperatures measured did represent within 0·1°C the sample temperatures. Also, the sample temperature was maintained constant within ±0·3°C in the temperature range investigated. Prior to each determination, the goniometer assembly was precisely aligned. The alignment was further verified by using an internal standard, silicon, of known unit-cell dimension and thermal coefficient of expansion.

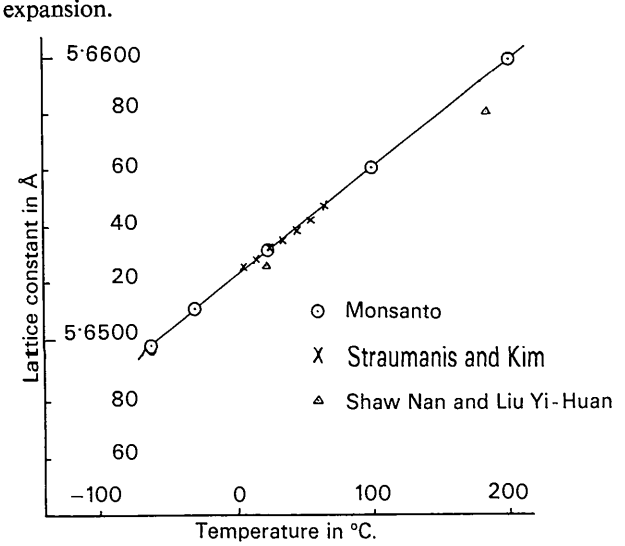

Fig. 1. Lattice parameters (Å) *versus* temperature.

The unit-cell dimension of GaAs was determined at −62, −30, 24, 100 and 200°C. The calculated lattice parameters were subjected to extrapolation according to the Nelson–Riley method (1945). At each temperature the 331, 422, 333, 620, 444 and 711 reflections were scanned. A scanning speed of 0·08° min^{-1}, corresponding to 5 inches of recorder chart travel per degree, permitted an accurate estimate of 2θ angle within 0·002. In the calculations, the following wavelengths were used in accordance with Lonsdale (1950): Cu $K\alpha_1 = 1{\cdot}54051$ Å and Cu $K\alpha_2 = 1{\cdot}54433$ Å.

In spite of the excellent distribution of points following a straight line relationship in the graphical procedure, the accuracy of the method is considered to be no better than ±0·0001 Å.

Fig. 1 shows the lattice parameters of GaAs plotted *versus* temperature. The published values of Straumanis & Kim (1965) and those of Shaw Nan & Liu Yi-Huan (1965) after conversion to Å are identified by crosses and triangles, respectively. The high degree of linearity of our data demonstrate the constancy of the thermal coefficient of expansion within the range of temperature investigated. Also, it indicates the excellent agreement with the results of Straumanis & Kim.

The linear thermal coefficient of expansion α was calculated following the relation:

$$\alpha = \frac{1}{a} \cdot \frac{\partial a}{\partial t} \qquad (1)$$

where a is the unit-cell dimension, taken as 5·6532 at 24°C. The value of the expansion coefficient is $\alpha = 6{\cdot}86 \times 10^{-6} \pm 0{\cdot}13 \times 10^{-6}°C^{-1}$. We consider this to be in good agreement with the previously reported value of $\alpha = 6{\cdot}4 \times 10^{-6}°C^{-1}$ by Straumanis & Kim (1965).

Table 1 shows the lattice constants of GaAs at the temperatures investigated.

Table 1. *Lattice constant* (*a*) *of* GaAs

Temperature	*a*
−62°C	5·6498
−30	5·6511
24	5·6532
100	5·6561
200	5·6600

References

LONSDALE, K. (1950). *Acta Cryst.* **3**, 400.

NELSON, Y. B. & RILEY, D. P. (1945). *Proc. Phys. Soc.* **57**, 160.

SHAW NAN & LIU YI-HUAN (1965). *Sci. Sinika* (*Peking*), **14**, 1582.

STRAUMANIS, M. E. & KIM, C. D. (1965). *Acta Cryst.* **19**, 256.