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Lattice Parameters and Thermal Expansion of Zinc Telluride and Mercury Selenide

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The lattice parameters of zinc telluride and mercury selenide were measured with a Unicam 19 cm high-temperature powder camera; the following equations represent the results: ZnTe, $a_t = 6{\cdot}1016 + 54{\cdot}63 \times 10^{-6}t + 6{\cdot}82 \times 10^{-9}t^2 + 5{\cdot}28 \times 10^{-12}t^3$; HgSe, $a_t = 6{\cdot}0854 + 28{\cdot}61 \times 10^{-6}t + 4{\cdot}93 \times 10^{-9}t^2 + 3{\cdot}74 \times 10^{-12}t^3$. The expressions for thermal expansion coefficients are also given.

Introduction

Previous work on the microscopic thermal expansion of zinc telluride and mercury selenide has not been very extensive. Novikova & Abrikosov (1963) determined the macroscopic thermal expansion of zinc telluride (sphalerite type structure) from 20 to 340°K with a silica dilatometer. They showed that the thermal expansion, α, changes sign at 46°K. Zhdansova, Lukina & Novikova (1966) measured the coefficient of thermal expansion of mercury selenide in the temperature range 20° to 500°K with a quartz type of dilatometer. The microscopic data of thermal expansion of zinc telluride at elevated temperatures have been published by Holland & Beck (1968) who determined the lattice parameters without the use of any graphical or analytical methods, which certainly gives better results. In the present investigations we have used a 19 cm Unicam High-Temperature Powder Camera. The lattice parameters were calculated by Cohen's (1936) analytical method with Nelson & Riley's (1945) extrapolation function.

Experimental

For diffraction work, fine quartz capillaries of inner diameter 0·3 mm were chosen. At each temperature the photographs were taken three times and care was taken to reproduce the same temperature within ±2°C. The methods of calibration of the thermocouple and evaluation of lattice parameters and thermal expansion coefficients were the same as those described by Singh (1968).

Results and discussion

Zinc telluride

Ultra-pure zinc telluride was annealed at 256°C for four hours and the well-resolved lines corresponding to reflexions 711, 642, and 731 (Cu $K\alpha$ radiation) were used for the derivation of the lattice parameters. These are tabulated in the first column of Table 1 and are expressed by the parabolic equation:

$$a_t = 6{\cdot}1016 + 54{\cdot}63 \times 10^{-6}t + 6{\cdot}82 \times 10^{-9}t^2 + 5{\cdot}28 \times 10^{-12}t^3 ,$$

where a_t is the lattice parameter in Å at t°C. The expression for the thermal expansion coefficient α_t is given by:

$$\alpha_t = 8{\cdot}95 \times 10^{-6} + 2{\cdot}24 \times 10^{-9}t + 2{\cdot}60 \times 10^{-12}t^2 .$$

Table 1. *Lattice parameters and thermal expansion coefficients of zinc telluride*

Temperature (°C)	Lattice parameter, a(Å) Observed	Calculated	$\alpha \times 10^6$ (°C^{-1})
35	6·1035	6·1035	9·03
103	6·1073	6·1073	9·21
167	6·1109	6·1109	9·40
256	6·1161	6·1161	9·70
352	6·1218	6·1219	10·06
445	6·1277	6·1278	10·46

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From our results, the value of the lattice parameter at 20 °C is 6·1026 Å. This compares with the values 6·085 (Horak, Machovec & Kosek, 1957), 6·102 (Zachariasen, 1926), 6·1026 (Swanson, Morris, Evans & Ulmer, 1964) and 6·1026 at 23 °C (Holland & Beck, 1968).

From the graph given by Novikova & Abrikosov (1963) the thermal-expansion coefficient at 27 °C is $8{\cdot}5\times10^{-6}\,°C^{-1}$ and our value is $9{\cdot}03\times10^{-6}\,°C^{-1}$ at 35 °C. The mean thermal expansion determined from the data of Holland & Beck (1968) is $9{\cdot}2\times10^{-6}\,°C^{-1}$ from 23 to 458 °C whereas our value is $9{\cdot}67\times10^{-6}\,°C^{-1}$ from 35 to 445 °C.

Mercury selenide

Pure mercury selenide was annealed at 150 °C for three hours. The reflexions 711, 642, and 731 were used for the derivation of the lattice parameters. The lattice parameters and the thermal expansion coefficients are given by the equations:

$$a_t = 6{\cdot}0854 + 28{\cdot}61\times10^{-6}t + 4{\cdot}93\times10^{-9}t^2 + 3{\cdot}74\times10^{-12}t^3$$

and

$$\alpha_t = 4{\cdot}70\times10^{-6} + 1{\cdot}62\times10^{-9}t + 1{\cdot}84\times10^{-12}t^2$$

respectively. Some values are given in Table 2.

Table 2. *Lattice parameters and thermal expansion coefficients of mercury selenide*

Temperature (°C)	a (Å) Observed	a (Å) Calculated	$\alpha\times10^6$ ($°C^{-1}$)
34	6·0864	6·0864	4·76
150	6·0898	6·0898	4·99
215	6·0919	6·0918	5·13
265	6·0934	6·0934	5·26
330	6·0954	6·0955	5·44
377	6·0971	6·0971	5·57

The room-temperature lattice parameter determined by Cruceanu, Nistor & Niculescu (1966) is $a=6{\cdot}088$ Å, by Bethke (1956) $a=6{\cdot}073$ Å and by Swanson, Gilfrich & Cook (1957) $a=6{\cdot}085$ Å; our value is $a=6{\cdot}0864$ Å at 34 °C.

Zhdansova *et al.* (1966) determined the thermal expansion of mercury selenide dilatometrically from 20 to 500 °K and they have plotted the thermal expansion coefficient against temperature. The value taken from their graph is about $1{\cdot}4\times10^{-6}\,°C^{-1}$ at 27 °C; our value at 34 °C is $4{\cdot}76\times10^{-6}\,°C^{-1}$ which is nearly three times greater than that of former workers. There seems to be some discrepancy here that needs investigation.

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Anomalous Neutron Scattering by Crystals and the Amplitudes of Vibration of Lattice Waves

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This paper deals with the scattering of neutrons by crystals which contain at least one anomalous scatterer. It is shown that anomalous scattering studies provide a powerful method of evaluating the amplitudes of lattice waves for crystals like CdS with at least one anomalous scatterer in the unit cell.

1. Introduction

It is well known that anomalous-dispersion methods provide a powerful tool for the phase determination of complex structures by X-ray scattering. If the nuclear resonance energies in a crystal are low and lie in the thermal neutron range, as in the case of substances like ^{113}Cd, ^{151}Eu, ^{149}Sm, and ^{157}Gd, strong anomalous-