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# Structures of 24 New Polytypes of Tin Disulphide*


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**Abstract.** The structures of 24 new polytypes of $SnS_2$ obtained from a vapour phase are presented: $8H_1$: $(f2f1)_2/(211)_2$ (*t–o–f*/Zhdanov notations); $10H_2$: $f2of1f2f1/2(11)_2211$; $12H_1$: $tf5tf1of1/22122111$; $12H_2$: $f2(o)_2f1f2f1/2(11)_3211$; $14H_2$: $f2(o)_2f1f2of1/2(11)_32(11)_2$; $22H_1$: $(f5f1f1)_3(t)_2/22(2121)_3$; $24H_1$: $f5f1f1f2f2f1f1f5f1f1(t)_2/2221212111212121$; $40H_2$: $(f5f1f1)_6(t)_2/22(2121)_6$; $42H_1$: $(f1f5f1)_6(o)_3/(2121)_6(11)_3$; $44H_1$: $(f1f5f1)_3o(f1f5f1)_2(o)_2f1f5f1o/(2121)_311(2121)_2(11)_2212111$; $24R_2$: $f2f2f1f1/211121$; $30R_2$: $f5f1f1(t)_2/222121$; $36R_1$: $f1f5f1(o)_3/2121(11)_3$; $42R_2$: $f5f1f1f2f2f1f1/2121211121$; $48R_2$: $(f5f1f1)_2(t)_2/22(2121)_2$; $54R_1$: $f1f5f1of1f5f1(o)_2/2121112121(11)_2$; $72R_1$: $f5f1f1f2f2f1of1(f2f1)_2/212121112111211211$; $84R_2$: $(f1f5f1)_2(f1f5f1o)_2/(2121)_2(212111)_2$; $96R_1$: $(f1f5f1)_3(o)_2f1f5f1(o)_2/(2121)_3(11)_22121(11)_2$; $96R_2$: $(f1f5f1)_3of1f5f1(o)_3/(2121)_3112121(11)_3$; $114R_1$: $(f1f5f1o)_4f1f5f1/(212111)_42121$; $132R_2$: $(f1f5f1o)_3(o)_4f1f5f1(o)_3/(212111)_3(11)_42121(11)_3$; $138R_1$: $(f5f1f1)_7(t)_2/22(2121)_7$; $144R_1$: $(f1f5f1o)_2(f1f5f1)_2of1f5f1(o)_6/(212111)_2(2121)_2112121(11)_6$.


**Experimental.** Crystals of $SnS_2$ were grown from vapour phase by the method of chemical transport. Starting materials were $SnS_2$ and $SnI_4$ powders, temperature of crystallization was in the range 670–1170 K (Pałosz, Pałosz & Gierlotka, 1984). Crystals – platelets from $1 \times 1 \times 0{\cdot}01$ to $10 \times 20 \times 0{\cdot}1$ mm – examined by X-rays in cylindrical camera with 43 mm radius and 0·7 mm collimator. Oscillation method with $a^*$ axis as rotation axis and with angle between incident beam (Co $K$ radiation) and $c$ axis varying between 15 and 30°. The method used here for the determination of the structures of 24 new polytypes of $SnS_2$ is similar to that described previously and used for $CdI_2$ and $SnS_2$ polytypes (Pałosz, 1982; Pałosz, Pałosz & Gierlotka, 1985). This method is based on the comparison of the experimental and theoretical intensity diagrams prepared for $10.l$ and $1\bar{1}.l$ reflexions where $1{\cdot}5 \le l/N \le 2{\cdot}5$ and $N$ is the number of S layers in a polytype cell. In the analysis of the theoretical models of the polytype cells formulae found for structural series were used (Pałosz, 1982; Pałosz *et al.*, 1985). For each polytype under investigation calculations of reflexion intensities were performed for a certain number of theoretical models: for a few models for simple polytypes (*e.g.* $8H$, $10H$, $22H$, $30R$) and up to about 20 models for complicated polytypes (*e.g.* $24H_1$, $44H_1$, $132R_2$, $144R_1$). The diagrams presented in Figs. 1–24 compare the measured values of reflexion intensities with those calculated for models corresponding to the identified polytypes of $SnS_2$.† The temperatures of growth of these polytypes are given in Table 1, where the polytype

* *Editorial note:* The Zhdanov notation used in this and the two following papers is a simplified version of the recommendations approved by the International Union of Crystallography *Ad-Hoc* Committee on the Nomenclature of Disordered, Modulated and Polytype Structures [Guinier, Bokij, Boll-Dornberger, Cowley, Ďurovič, Jagodzinski, Krishna, de Wolff, Zvyagin, Cox, Goodman, Hahn, Kuchitsu & Abrahams (1984). *Acta Cryst.* A**40**, 399–404].

† Figs. 1–24 and tables listing calculated and observed intensities for $SnS_2$ polytypes have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42251 (37 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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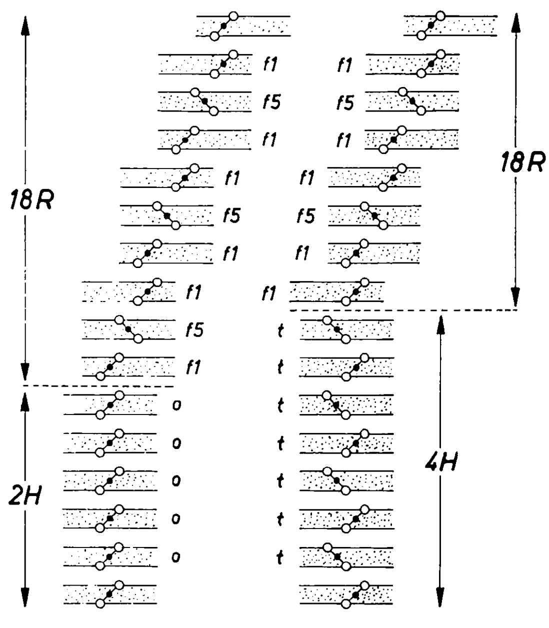
Table 1. *Structure and growth conditions of 24 polytypes of tin disulphide*

| Ramsdell* symbol | *t–o–f* notation | Temperature of growth (K) |
|---|---|---|
| Hexagonal polytypes | | |
| $8H_1$ | $(f2f1)_2$ | 875 |
| $10H_2$ | $f2f1f2of1$ | 800 |
| $12H_1$ | $tf5f1of1$ | 840 |
| $12H_2$ | $f2f1f2(o)_2f1$ | 880 |
| $14H_2$ | $f2of1f2(o)_2f1$ | 860 |
| $22H_1$ | $(f5f1f1)_3(t)_2$ | 840 |
| $24H_1$ | $f5f1f1f2f2f1f1f5f1f1(t)_2$ | 1015 |
| $40H_2$ | $(f5f1f1)_6(t)_2$ | 1015 |
| $42H_1$ | $(f1f5f1)_6(o)_3$ | 875 |
| $44H_1$ | $(f1f5f1)_3o(f1f5f1)_2(o)_2f1f5f1o$ | 925 |
| Rhombohedral polytypes | | |
| $24R_2$ | $f2f2f1f1$ | 885 |
| $30R_2$ | $f5f1f1(t)_2$ | 1015 |
| $36R_1$ | $f1f5f1(o)_3$ | 800 |
| $42R_2$ | $f5f1f1f2f2f1f1$ | 675 |
| $48R_2$ | $(f5f1f1)_2(t)_2$ | 1015 |
| $54R_1$ | $f1f5f1of1f5f1(o)_2$ | 860 |
| $72R_1$ | $f5f1f1f2f2f1of1(f2f1)_2$ | 875 |
| $84R_2$ | $(f1f5f1)_2(f1f5f1o)_2$ | 1015 |
| $96R_1$ | $(f1f5f1)_3(o)_2f1f5f1(o)_2$ | 875 |
| $96R_2$ | $(f1f5f1)_3of1f5f1(o)_3$ | 875 |
| $114R_1$ | $(f1f5f1o)_4f1f5f1$ | 1115 |
| $132R_2$ | $(f1f5f1o)_3(o)_4f1f5f1(o)_3$ | 875 |
| $138R_1$ | $(f5f1f1)_7(t)_2$ | 1015 |
| $144R_1$ | $(f1f5f1o)_2(f1f5f1)_2of1f5f1(o)_6$ | 875 |

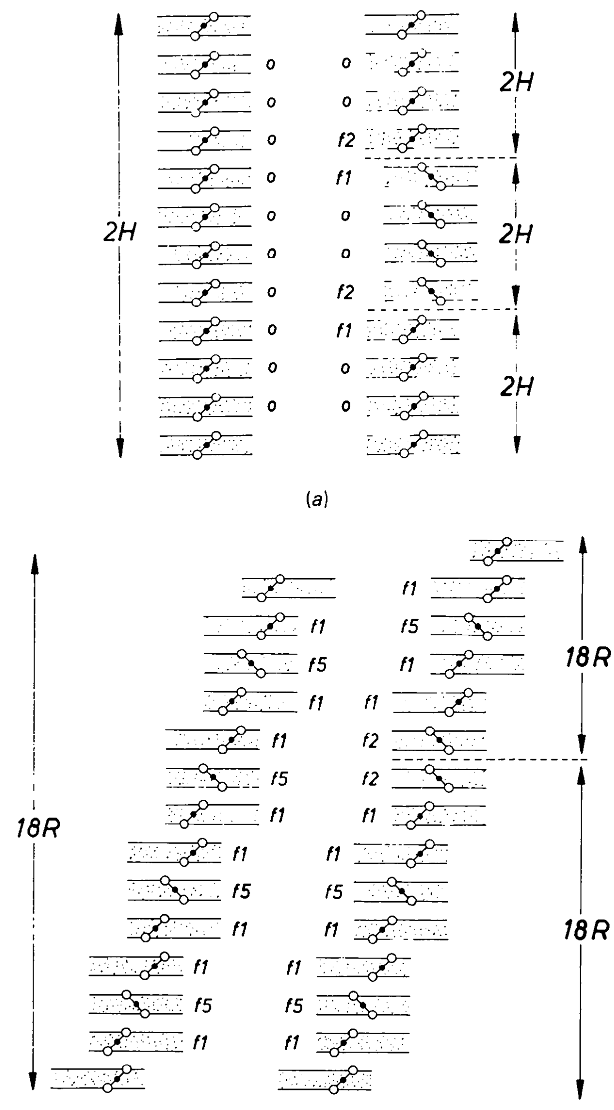
* Indices of Ramsdell symbols are after Pałosz *et al.* (1985).

cells are described in the *t–o–f* notation (Pałosz, 1982). Some discrepancies between the experimentally measured and theoretically calculated intensities are observed in Figs. 1–24 for several polytypes. They occur in the cases when reflexions of a polytype are superimposed with reflexions of basic polytypes $2H(8H_1, 36R_1, 144R_1)$, $4H(12H_1, 24H_1, 54R_1)$ or $18R(24H_1, 42H_1, 48R_2)$ or when a polytype occurs with a superimposed disorder, *e.g.* $8H_1$, $12H_2$, $24H_1$, $40H_2$, $42H_1$, $30R_2$, $54R_1$, $96R_1$, $114R_1$, $138R_1$. In these cases the measured intensities are not considered to be very reliable but the small discrepancies observed in Figs. 1–24 are not important for a unique structure identification when one uses intensity diagrams (Pałosz, 1982).




(*a*) (*b*)

Fig. 25. Arrangement of molecules *X–M–X* in the plane (11.0) (zig-zag sequence) in the interface between (*a*) 2*H*- and 18*R*-type sequences, (*b*) 4*H*- and 18*R*-type sequences.




(*b*)

Fig. 26. Multidomain structures (*a*) 2*H* and (*b*) 18*R* with the sequences $f1f2$ and $f2f2$ in the interdomain interfaces.

**Discussion.** Recently 21 polytypes of $SnS_2$ were reported and a multiphase model for characterization of their structures was suggested (Pałosz *et al.*, 1985). The structural series of polytypes with intermediate structures $2H$–$18R$, $4H$–$18R$ and $2H$–$4H$–$18R$ were derived theoretically with the use of a multiphase model of polytype structures (Pałosz, 1983) and only polytypes of these three kinds were found in $SnS_2$ crystals. Most of the polytypes presented here also belong to these three main structural groups: $2H$–$18R$: $42H_1$, $44H_1$, $36R_1$, $54R_1$, $84R_2$, $96R_1$, $96R_2$, $114R_1$, $132R_2$ and $144R_1$; $4H$–$18R$: $22H_1$, $40H_2$, $30R_2$, $48R_2$, $138R_1$; $2H$–$4H$–$18R$: $12H_1$. Besides these simple polytypes some polytypes were found to have a more complicated composition: they contain the stackings of layers not belonging to basic structures $2H$ (stackings $o$), $4H$ ($t$) or $18R$ ($f1f5f1$), namely $f1f2$ ($8H_1$, $10H_2$, $12H_2$, $14H_2$) or $f2f2$ ($24H_1$, $24R_2$, $42R_2$, $72R_1$). The stackings of layers (zig-zag sequences of S–Sn–S molecules) corresponding to simple mixed structures $2H$–$18R$ and $4H$–$18R$ are presented in Fig. 25. As has already been seen, structures of this kind may be considered to be composed of domains of pure basic structures. Here each molecular layer belongs to one of the simple phases: $o,t,f1f5f1$. Note that in this case no faulted arrangements of layers occur in the interphase interfaces. Fig. 26 presents the stackings $f1f2$ and $f2f2$ found in polytypes of $SnS_2$. These two 'faulted sequences' may be considered as a kind of interdomain boundary occurring between neighbouring domains of the same structure: faults $f1f2$ occur in the $2H$–$2H$ interface (between the domains $2H$ having different orientations of molecules); faults $f2f2$ occur in the multidomain structure $18R$. Note that the structures presented in Fig. 26 are similar to the multidomain structure $4H$ called structure $D$ and occurring frequently in $CdI_2$ and $PbI_2$ crystals (Pałosz, 1983). The layers $f1$ and $f2$ occur frequently in polytypes of $CdI_2$ and $PbI_2$ and, as discussed elsewhere (Pałosz, 1983), these layers were found to be interdomain boundaries between domains $2H$ and $4H$. The same layers occurring in $SnS_2$ polytypes, however, can in no case be regarded as $2H$–$4H$ boundaries. The $2H$ and $4H$ polytypes occur in $SnS_2$ as in $CdI_2$ and $PbI_2$, but no polytypes were found to be constructed of domains $2H$ ($o$ layers) and $4H$ ($t$) with layers $f1$ and $f2$ occurring between the domains.

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# Polytypism of $SnSe_2$ Crystals Grown by Chemical Transport: Structures of Six Large-Period Polytypes of $SnSe_2$


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**Abstract.** The polytype structure of $SnSe_2$ single crystals grown by chemical transport is examined by X-rays. Frequencies of occurrence of different polytype structures are given and structures of six large-period polytypes are identified: $12H_1$: $f2(o)_2f1f2f1$/ $2(11)_3211$ ($t$–$o$–$f$/Zhdanov notations); $48H_1$: $(f1f5f1)_4[f1f5f1(o)_3]_2/(2121)_4[2121(11)_3]_2$; $24R_1$: $f1f5f1o/212111$; $24R_2$: $f2f2f1f1/211121$; $30R_1$: $f2of2f1f1/2(11)_2121$; $54R_1$: $f2(o)_5f2f1f1/2(11)_6$-$121$.

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