electronic grade CdS by thermal evaporation under vacuum (1.3×10^{-4} Pa) on glass slides which were precooled to liquid-nitrogen temperature. The films employed in the present investigation had thicknesses ranging from 200 to 700 Å. The crystallographic characterization was done by employing electron microscope techniques – in both imaging and diffraction modes. It was found that the initial phase of the film was amorphous. On undergoing an amorphous to crystalline transformation brought about by annealing the amorphous films up to a temperature of about 773 K by employing a focused electron beam for 10 to 30 s, single-crystal regions were formed. The annealing temperature was ascertained from a precalibration of the electron beam (Srivastava & Srivastava, 1975). After cooling the sample almost to room temperature the diffraction patterns were recorded from the single-crystal regions. The diffraction pattern which was most often observed corresponded to a hexagonal phase with $a = 4.15$ and $c = 6.72$ Å. This is compatible with the known $2H$ phase. Although the electron diffraction intensities are not very accurate, intensity data collected from several patterns suggested that this phase has the known wurtzite-type structure. Very often diffraction patterns were found which were unequivocally explicable based on the same periodicity in the a direction as that of $2H$ but with the periodicity in the direction of c being double and triple that of $2H$, *i.e.* $c = 13.44$ and $c = 20.16$ Å. Thus, apart from $2H$, the polytypes $4H$ and $6H$ were also stabilized as a consequence of the amorphous to crystalline transformations. Besides these, some other polytypes with high periodicity whose identity could not be definitely established were also obtained. The determination of the stacking sequence (structure) for none of these polytypes was attempted. The foregoing polytypes, when once formed, did not transform to any other structure on annealing at high temperatures and thus they represented stable phases.

In order to explore the high-temperature transformation characteristics of the initial amorphous films, annealing was also done at high temperatures $773 \leq T \leq 1173$ K. This mode of annealing was found to yield two different modifications: both of these were hexagonal and had the same periodicity along **a** ($a = 5.12$ Å). The periodicities along **c** were 8·62 and 21·50 Å. The most commonly occurring modification (high-temperature modification) was the one with $c = 8.62$ Å. Taking this to correspond to the phase with the minimum number of layers in the unit cell, it can be designated as $2H_1$. The other modification is $5H_1$. Some other polytypes in this category were disordered. Preliminary observations carried out by us on other cadmium chalcogenides revealed that the occurrence of polytypism in thin films is a general phenomenon. Thus, when amorphous cadmium telluride thin films transform to the crystalline phase, several polytypes are found to result.

In conclusion, it can be said that several new polytypes have been found to exist in cadmium sulphide thin crystals. These represent the first reported polytypes of cadmium sulphide. As regards the mechanism of formation, in view of the special mode of stabilization of polytypes, as a consequence of amorphous to crystalline transformation, none of the known mechanisms (Baronnet, 1978) can directly explain the genesis of CdS polytypes. It appears that a new possible mechanism will have to be worked out to make the formation of the present polytypes intelligible. Attempts are being presently made to put forward a feasible mechanism and results will be forthcoming.

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Commission on Journals

Standards for the Publication of Powder Pattern Data

Standards for the publication of powder patterns, originally compiled by a subcommittee of the American Crystallographic Association and published in *National Bureau of Standards Special Publication* 567 (1979), have been accepted by the Commission on Crystallographic Data and the Commission on Journals. Papers that present powder pattern data submitted for publication in IUCr journals are now required to follow these standards.

The information requested by the standard data-form, a completed example of which is given in Table 1, must be given as compactly as possible. Essential information is requested by the bold-face headings. The remaining information sought is highly desirable, although it is recognized that some may not be available in all cases. Partial omission of the optional data will not preclude publication of the paper. Powder data corresponding to the information given in Table 1 are presented, in the preferred form, in Table 2. Reprints of the complete standard, including copies of the blank data-form, are available from any Co-editor. Guidance in filling out the form is available from the JCPDS International Center for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081, USA.

Among the requirements for reporting powder diffraction data are:

(*a*) The published powder pattern should be as complete as possible and should include weak as well as strong diffraction lines. Where possible, the data should extend to at least 100° 2θ (Cu $K\alpha$ radiation). Patterns with a small number of lines should extend to the limit of the experimental method used.

(*b*) The experimentally observed 2θ values should be given in degrees, corrected for systematic instrumental error.

(*c*) Intensities should be reported numerically, with the most intense line scaled to 100 and intensities less than 1 reported as decimal fractions. Intensity values reported should not imply a precision greater than that measured.

(*d*) The reproducibility of the measured values of 2θ and I should be indicated, as obtained by multiple mountings of the sample material.

(*e*) Indexing of the powder diffraction data is required for all but the rarest and best-defended cases. Authors should report a figure of merit based on the accuracy of the 2θ measurements and the completeness of their data.

(*f*) Information concerning line breadth of the sample should be supplied.

(*g*) Additional information of value to future users should be supplied, such as the standard deviations, Chemical Abstracts Service Registry number, Crystal Data index number, *etc.*

To justify being published, powder diffraction data must constitute an original contribution to the literature. As an original contribution, the data must be the first published for a well-characterized phase, must be a significant correction to or an improvement on published data, or must relate to the phase in a previously uncharacterized condition, *e.g.* at elevated temperature or pressure. A powder pattern calculated from single-crystal structure data does not in itself meet the criterion of originality.

Table 1. *Example of completed data form: powder diffraction data for phase characterization*

Data from Swanson, H. E. *et al.* (1971). *NBS Monograph* No. 25, Section 9, p. 25.

Bold-face items are considered essential.

Sample characterization

Name (chemical, mineral, Trivial) Magnesium aluminum oxide (spinel)
Empirical formula $MgAl_2O_4$
Chemical analysis No × Yes
Source/preparation Synthetic; fusion of binary oxides

Chemical Abstracts Registry No. 12068·51·8
Pearson phase designation cF56
Other **Index of Refraction = 1·718 (Isotropic)**

Technique

Radiation type, source X-rays, Cu λ value used 1·54056 Å $K\alpha_1$
λ Discrim. (Filters, mono, *etc.*) Diffracted beam, curved LiF mono
λ Detector (Film, Scint., Position-sensitive, *etc.*) Geiger
Instrument description (Type, Slits, *etc.*) 17 cm vertical diffractometer
Div 1° Rec 0·003″
Soller Yes No. 1 Position Inc. Aperture q = 1·2
Instrumental profile breadth 0·10 °2θ Temp. (°C) 25 ± 1
Specimen form/particle size
Edge loaded powder/< 10 μm particle size for I's, packed for 2θ's
Range of 2θ from 5 °2θ to 165·0 °2θ Specimen motion None
Internal/external 2θ std (if any) Ag (internal)
Lattice parameter of 2θ std 4·08641 Å
2θ error correction procedure Linear interpolation from nearest 2θ's of std.
Intensity meas. technique Strip chart record (peak heights)
Error (~) 5% Peak × Integrated
Minimum intensity threshold (in relative intensity units) 0·3
Intensity std used α-Al_2O_3 *hkl*'s of intensity std 113
Intensity ratio I/I_c 1·70 (5) Conversion factor if corundum not used
Resolution (FWHM) for this material: 0·10 °2θ at 59·37 °2θ
2θ reproducibility for this material: ±0·02 °2θ at All °2θ

Unit-cell data

Method of cell detn. Cell and structure known from Bragg (1915)
Cell refinement method Least-squares. See Appleman & Evans (1973)
a = 8·0831 (1) Å; b = ( ) Å; c = ( ) Å
α = ° (°); β = ° (°); γ = ° (°)
Z = 8; D_m = ( ) Mg m^{-3}; D_x = 3·578 Mg m^{-3}; V = 528·1 $Å^3$;
Formula Wt. = 142·25
Crystal sys. Cubic Space group *Fd*3*m* [227]
Crystal data index No. 8·0831
Figure of merit type F_N. See Smith & Snyder (1979)
Value F_{29} = 58 (0·015, 33)

References

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( ) indicates standard deviation in least significant digit(s).

Table 2. *Presentation of powder data*

Information in the first two columns is essential, that in the remaining three columns is desired (see text).

2θ exp (°)	I/I_0	d_{exp} (Å)	*hkl*	$\Delta 2\theta$* (°)
19·02	35	4·66	111	+0·019
31·27	40	2·858	220	−0·003
36·84	100	2·437	311	−0·009
38·53	3	2·335	222	−0·021
44·83	65	2·020	400	+0·016
55·64	9	1·650	422	−0·020
59·37	45	1·5554	511	+0·008
65·24	55	1·4289	440	−0·001
68·64	3	1·3662	531	+0·006
74·13	3	1·2780	620	+0·003
77·32	8	1·2330	533	−0·029
78·40	1	1·2187	622	−0·013
82·64	5	1·1666	444	+0·006
85·76	2	1·1320	711	−0·012
90·97	5	1·0802	642	−0·009
94·10	12	1·0524	731	−0·005
99·34	7	1·0104	800	−0·006
107·90	2	0·9527	822	−0·020
111·22	8	0·93343	751	−0·014
112·32	1	0·92738	662	−0·035
116·91	6	0·90384	840	−0·025
120·50	1	0·88722	911	+0·004
121·69	0·9	0·88203	842	−0·021
126·76	0·8	0·86161	664	+0·013
130·74	8	0·84737	931	−0·011
138·07	17	0·82488	844	+0·033
142·97	0·4	0·81232	933	+0·024
152·70	2	0·79266	10,2,0	−0·033
160·65	11	0·78139	951	+0·025

* $2\theta_{exp} - 2\theta_{calc}$.