ploy them is in eliminating incorrect atomic positions. To formulate, however, the best possible criteria with the R_2 or D function is not yet possible, because the distribution functions $P(R_2)$ or $P(D)$ are still unknown.

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Polytypism in Silver Iodide

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Synthetic crystals of silver iodide are shown to form polytypes other than the previously reported wurtzite-type β-AgI and sphalerite-type γ-AgI. Four new polytypes have been discovered and their layer sequences determined by X-ray diffraction. The constant of proportionality between percentage hexagonality and birefringence of AgI polytypes has been established.

Introduction

Silver iodide is reported to be trimorphic at atmospheric pressure (*e.g.* Burley, 1963*a*). Below a transition temperature of 147 °C the structure may be of the sphalerite-type (γ-AgI) or the wurtzite-type (β-AgI). These transform to a body-centred cubic structure (α-AgI) in which the silver ions are disordered (Strock, 1934).

Single crystals of β-AgI have been grown by several methods: Helmholz (1935), Cochrane (1967), Mills, Perrott & Fletcher (1970), Suri, Henisch & Faust (1970). The most detailed investigation of the hexagonal form is due to Burley (1963*b*), and his crystallographic data are summarized as follows:

Space group $P6_3mc$
Cell dimensions $a_0=4{\cdot}592$, $c_0=7{\cdot}510$ Å
I at $(\frac{1}{3},\frac{2}{3},0)$, $(\frac{2}{3},\frac{1}{3},\frac{1}{2})$
Ag at $(\frac{1}{3},\frac{2}{3},u)$, $(\frac{2}{3},\frac{1}{3},\frac{1}{2}+u)$ with $u=0{\cdot}6253$
Isotropic temperature factors $B_{\rm I}=1{\cdot}8$, $B_{\rm Ag}=3{\cdot}4$ Å^2.

The very existence of the low-cubic polymorph γ-AgI has been disputed by Majumdar & Roy (1959). If it does exist it is almost certainly metastable at all temperatures below the $\gamma\rightarrow\alpha$ transition at 555 °C (Burley, 1963*a*). Fridrichsons & Mathieson (1962) have described γ-AgI as a metastable disordered polytype of β-AgI produced by crushing the latter. Certainly we are not aware of any successful attempts to grow single crystals of γ-AgI, and structural investigations of the β-AgI–γ-AgI system have been performed with powder samples only (Bloch & Möller, 1931; Manson, 1956; Majumdar & Roy, 1959; Burley, 1963*a*, 1964). Conflicting conclusions have been drawn from these studies concerning the stability relations between the putatively coexisting γ and β forms. Bloch & Möller (1931) found that the sphalerite form was stable at low temperatures and they imply an equilibrium transformation $\gamma\rightleftharpoons\beta$ at about 135 °C. Manson (1956) reports that the transition $\gamma\rightarrow\beta$ occurred rapidly at all temperatures above 120 °C and that the transformation was partially reversible. Burley (1963*a*, 1964) found that the phase change was irreversible under ordinary conditions. Significantly Majumdar & Roy (1959) while discounting the equilibrium transition $\gamma \rightleftharpoons \beta$ and disputing the existence of a pure sphalerite form of AgI found evidence of several complex (but unspecified) polytypes.

It is our purpose to provide evidence from single-crystal structural studies confirming the claims of Majumdar & Roy (1959) that low AgI occurs in a number of different polytypic modifications and to report four new structural forms of AgI. We also report birefringence measurements that may be useful in determining the structures of higher-order polytypes.

Experimental

The crystals in this investigation were grown by the method of Cochrane (1967) which involves the slow diffusive dilution of a solution of AgI in concentrated aqueous KI solution. This method of growth produces hexagonal pyramids or hexagonal prisms, the latter growing to several cm in length and a few mm in diameter. For X-ray studies however it is convenient to select quite fine hexagonal prismatic needles: the finest of these may be less than 0·1 mm in diameter and up to 0·5 cm long. For crystals thicker than ~0·5 mm absorption becomes prohibitive if the crystal is immersed in the incident beam and it is then preferable to observe reflexions from the extended crystal faces.

Some 40 crystals were investigated by X-ray diffraction in this series and the new polytypes were identified (as discussed below) from zero-level $(H0.L)$ precession photographs obtained with Mo $K\alpha$ or Cu $K\alpha$ radiation. When the resolution of neighbouring reflexions was in any doubt the periodicities of the structures were confirmed by *a*-axis Laue photography.

Description of polytypes

Both in the low-cubic and the hexagonal modifications of AgI, as in the isomorphs of SiC and ZnS, the atoms of each species are tetrahedrally bonded to four unlike nearest-neighbour atoms, and the structures can be pictured as two interpenetrating close-packed arrays of atoms. The wurtzite-type structure corresponds to hexagonal close packing *ABAB*... along hex. [00.1], the sphalerite-type structure to cubic close packing *ABCABC*... along f.c.c. [111]. All other polytypes correspond to mixed stacking sequences.

The relationship between a given Ag–I layer *A*, *B* or *C* and its predecessor is specified by + or − in the Hägg notation. The + represents a translation $(+\frac{1}{3}, +\frac{2}{3})$ in the basal plane and thus the cyclic relationships $A \rightarrow B \rightarrow C \rightarrow A$; the − represents a translation $(-\frac{1}{3}, -\frac{2}{3})$ and thus the anticyclic relationships $A \rightarrow C \rightarrow B \rightarrow A$. The Ramsdell notation is used to designate polytypes without implying the stacking sequence. Thus *nH*, *nR* or *nC* designates an *n*-layered hexagonal, rhombohedral or cubic polytype. When the detailed structures are known the stacking sequences of polytypes are compactly specified by the Zhdanov symbol consisting of pairs of numbers in which the first denotes the number of consecutive + signs, and the second the number of − signs, in the Hägg symbol. The Ramsdell zigzag sequence (which is the pictorial analogue of the Zhdanov symbol) can also be used to describe AgI polytypes: it shows the sequence of atoms in the $(11\bar{2}0)$ planes within which lie all the atoms of the structure. Details concerning these and other notations for describing polytypic structures can be found in Verma & Krishna (1966) and Trigunayat & Chadha (1971).

AgI polytypes

Crystals grown by Cochrane's method have been reported to conform to the wurtzite-type structure 2*H* (Cochrane, 1967). Cochrane found the density of stacking faults to be low and 'no evidence to suggest the presence of any low-temperature cubic structure'. Our studies show however that under similar conditions of growth the initial structure formed by AgI is 4*H* (Zhdanov symbol 22), and that the density of stacking faults (*i.e.* the random stacking disorder superposed on the ordered structure) is widely variable. Furthermore we have found that among crystals allowed to age at room temperature over a period of months the 4*H* structure occasionally transforms to longer period polytypes with increasing hexagonality culminating in the 2*H* end-member polytype. The 4*H* → 2*H* transformation also occurs on heating the crystals at ~100°C for a few minutes. In all, four new polytypes of AgI were discovered in this investigation. We designate them 4*H*, 8*H*, 12*H* and 16*H* in the Ramsdell notation.

Structure determination

The structure of the 4*H* polytype was uniquely determined once the periodicity was established, since 22 represents the only four-layered structure whose stacking sequence does not violate the condition that the first and last layers of the sequence be in different positions. This constraint may be expressed as

$$n_+ - n_- = 0 \pmod 3 \tag{1}$$

where n_+ and n_- are the numbers of + and − signs in the Hägg symbol.

The layer sequences of the remaining polytypes were determined by the following argument. It is known that for substances such as AgI, SiC or ZnS which crystallize in structures whose atoms lie in close-packed arrays the binary tetrahedral arrangement of atoms permits of only four possible space groups, *viz.* $P3m1$, $P6_3mc$, $R3m1$ and $F\bar{4}3m$ (Verma & Krishna, 1966). The latter two can be excluded from consideration here since the only polytype in space group $F\bar{4}3m$ is the end-member γ-AgI which we have not observed and all observed polytypes conformed to an hexagonal primitive Bravais lattice.

Were the number of layers odd the space group would be necessarily $P3m1$; however in all three cases there is an even number of layers and the space group may be either $P3m1$ or $P6_3mc$. It is necessary therefore to distinguish between structures which belong to the trigonal space group whose highest symmetry element is the triad axis, and those belonging to the hexagonal space group and possessing a hexad screw axis. Ordinarily the distinction is straightforward since the combination of a hexad with the apparent centre of symmetry that arises as a result of Friedel's law gives rise to an apparent mirror plane perpendicular to $\mathbf{c}^*$ in the reciprocal lattice. Then for structures with space group $P6_3mc$ the reflexions $hk.l$ and $hk.\bar{l}$ are equivalent (anomalous dispersion effects apart). For trigonal structures, by contrast, these reflexions are symmetrically situated about the zero layer line $\mathbf{a}^*$, but have quite different intensities in general. Ramsdell & Kohn (1951), however, discovered a trigonal polytype of silicon carbide, 10*H* (3223) which exactly simulated hexagonal symmetry. They demonstrated that the higher symmetry was simulated by structures of this type whenever the Zhdanov symbol or zigzag sequence of the trigonal polytype was itself symmetrical. The new AgI polytypes all show an apparent or real mirror plane perpendicular to $\mathbf{c}^*$: their space groups are therefore either $P6_3mc$ or $P3m1(s)$, where the parenthetic *s* denotes a symmetric Zhdanov symbol for the structure.

Verma & Krishna (1966) demonstrate that for an *n*-layered polytype in $P6_3mc$ the presence of the 6_3 axis requires that the stacking sequence from $n/2$ to n must be the reverse of the stacking sequence from 0 to $n/2$. This implies that the Zhdanov symbol for a polytype in $P6_3mc$ consists of an odd set of terms repeated. The converse is also true. (A symbol constituted by the repetition of an even set of terms represents either a sequence which violates the stacking constraint, equation (1), or a structure which repeats in $n/2$ layers. $2121 \equiv ABCBCA$ is an example of the former and $4141 \equiv ABCAB|ABCAB$ one of the latter.) For a polytype in $P3m1(s)$ the Zhdanov symbol consists of an odd or even *non-symmetrical* set of terms followed by the same set reversed. Again the converse is also true. (An odd *symmetrical* set followed by the same set reversed represents a structure in $P6_3mc$; an even *symmetrical* set, one that repeats in $n/2$ layers.)

It follows that for structures in $P6_3mc$ or $P3m1(s)$ the stacking sequence for the entire unit cell is determined by the sequence of half the unit cell. By analogy with the abbreviated notation $(a_1b_1a_2b_2 \ldots a_kb_k)_3$ used to represent the Zhdanov symbol for rhombohedral polytypes, wherein the entire stacking sequence is determined by one-third of the (hexagonal) unit cell, we can represent a polytype in $P6_3mc$ by the symbol $(a_1b_1\ldots)_2$ and a polytype in $P3m1(s)$ by $(a_1b_1\ldots)_{\bar{2}}$.

All possible Zhdanov symbols $(a_1b_1\ldots)_2$ and $(a_1b_1\ldots)_{\bar{2}}$ for 4*H*, 8*H*, 12*H* and 16*H* 'symmetrical' polytypes were enumerated. Although it was thought unlikely that the Zhdanov symbols for the AgI polytypes would contain terms other than 1's or 2's, this constraint was not imposed. Enumeration produced Table 1 which shows the number of unique structures possible. The expected Bragg intensities for all the structures represented by the Table 1 were calculated on an ICL 1904 A computer. Lorentz–polarization corrections and isotropic temperature factors (Burley, 1963*b*) were included, but corrections for absorption and anomalous dispersion were omitted from the calculations.

Table 1. *Number of unique structures possible for 'symmetric' polytypes*

Polytype	Zhdanov symbol contains only 1's and 2's	No restriction on the terms in the Zhdanov symbol
2*H*	1	1
4*H*	1	1
8*H*	2	4
12*H*	5	15
16*H*	14	62

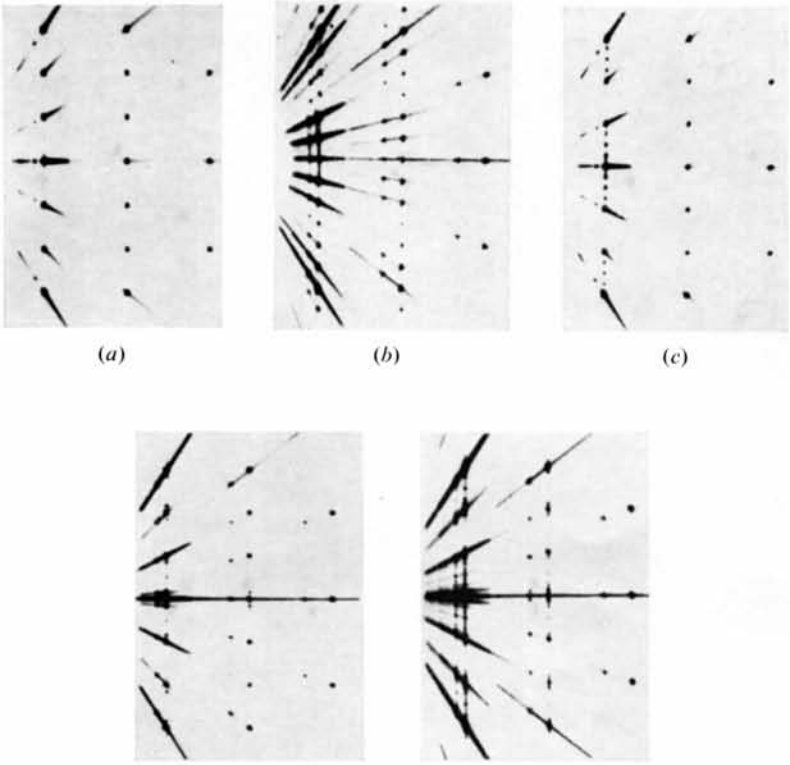
Fig. 1 shows portions of the zero layers of the reciprocal lattice obtained by X-ray precession photography of representative AgI specimens exhibiting the new forms of polytypism. Observed intensities on a relative scale were obtained by visual comparison of the film blackening due to reflexions along $10.l$ or $20.l$ lines. In all cases there was qualitative agreement between calculated and observed intensities for only one of the postulated structures or, in the case of the 12*H* polytype, structure combinations. A combination of two structures had to be considered for the latter since it was always found to occur in syntactic coalescence with the 2*H* structure. The structure of the 12*H* polytype was then identified by consideration of only those reflexions which do not coincide with 2*H* reflexions, *i.e.* reflexions $h0.l$ with $l \neq 0 \pmod 6$.

Table 2. *Structure and intensities of* 4*H polytype*

Space group	$P6_3mc$
Zhdanov symbol	22
Stacking sequence	*ABCB*
Percentage hexagonality	$\alpha = 50$
Unit-cell dimensions (Å)	$a_0 = 4{\cdot}592$, $c_0 = 15{\cdot}02$

$10.l$	I_{obs}	I_{calc}
0	*s*	429
1	*vs*	847
2	*s*	480
3	*w*	37
4	*m*	112
5	*s*	494
6	*vs*	1000
7	*m*	94
8	*abs*	1
9	*w*	52
10	*s*	308

Tables 2 to 5 summarize the structural details for each of the new AgI polytypes and compare observed and calculated intensities of $10.l$ reflexions. Calculated



(*a*) (*b*) (*c*)

(*d*) (*e*)

Fig. 1. Zero-level ($H0.L$) precession photographs of AgI polytypes, obtained with Mo radiation. (*a*) $2H$; (*b*) $4H$; (*c*) $8H$; (*d*) $12H+2H$ in syntactical coalescence; (*e*) $16H$.

Table 3. *Structure and intensities of* 8*H polytype*

Space group	$P3m1$
Zhdanov symbol	$211112=(211)_{\bar{2}}$
Stacking sequence	*ABCBCBCB*
Percentage hexagonality	$\alpha=75$
Unit-cell dimensions (Å)	$a_0=4\cdot592$, $c_0=30\cdot04$

10.l	I_{obs}	I_{calc}
0	*vvs*	693
1	*s*	269
2	*s*	195
3	*m*	108
4	*vs*	480
5	*abs*	3
6	*abs*	8
7	*w*	40
8	*vs**	181
9	*m*	106
10	*m*	114
11	*m*	102
12	*vvs*	1000

* The strength of I_{obs} indicates that the 8*H* polytype may be in syntactic coalescence with a small proportion of the 2*H* polytype.

Table 4. *Structure and intensities of* 12*H polytype*

Space group	$P6_3mc$
Zhdanov symbol	$2111121111=(21111)_2$
Stacking sequence	*ABCBCBCBABAB*
Percentage hexagonality	$\alpha=83\cdot3$
Unit-cell dimensions (Å)	$a_0=4\cdot592$, $c_0=45\cdot06$

10.l	I_{obs}	I_{calc}
0	[*vvs*]*	784
1	*s*	1000
2	*abs*	0
3	*m*	172
4	*abs*	0
5	*m*	284
6	[*vs*]	876
7	*vw*	35
8	*abs*	0
9	*abs*	7
10	*abs*	0
11	*m*	185
12	[*vs*]	205
13	*m*	346
14	*abs*	0
15	*w*	100
16	*abs*	0

* Observations in parentheses correspond to coincident 2*H* and 12*H* reflexions.

Table 5. *Structure and intensities of* 16*H polytype*

Space group	$P3m1$
Zhdanov symbol	$1121111111111211=(1121111)_{\bar{2}}$
Stacking sequence	*ABABCBCBCBCBCBAB*
Percentage hexagonality	$\alpha=87\cdot5$
Unit-cell dimensions (Å)	$a_0=4\cdot592$, $c_0=60\cdot08$

10.l	I_{obs}	$I_{\text{calc}}(1121111)_{\bar{2}}$	$I_{\text{calc}}(311111)_{\bar{2}}$
0	$vs>8$	1000	1000
1	$vs\leq8$	898	300
2	*m*	143	172
3	$w>5$	21	78
4	*m*	104	79
5	*w*	14	143
6	$w>5$	57	192
7	*m*	212	173
8	*vs*	960	581
9	*w*	46	38
10	*abs*	2	6
11	*abs*	0	1
12	*abs*	4	3
13	*abs*	2	7
14	*w*	21	25
15	*m*	183	61
16	*s*	261	261

intensities were normalized so that the strongest reflexion has $I_{\text{calc}}=1000$. Table 5 includes the intensities calculated for the 'next best' 16*H* structure, Zhdanov symbol $(311111)_{\bar{2}}$. There is fair agreement between I_{obs} and I_{calc} for this structure but some discrepancies are apparent and this structure can be therefore rejected in favour of $(1121111)_{\bar{2}}$.

Birefringence of AgI polytypes

The values of the percentage hexagonality α quoted in Tables 2 to 5 were obtained from the relation (Brafman, Alexander & Steinberger, 1967):

$$2k=\alpha n/100 \qquad (2)$$

where $2k$ is the number of elements in the Zhdanov symbol and n is the number of layers in the unit cell. α is defined (Brafman & Steinberger, 1966) as the percentage of close-packed planes which are in a hexagonal nearest-neighbour environment. For the 2*H* structure $\alpha=100$, for the 3*C* $\alpha=0$. The percentage hexagonality is an important parameter in that several physical properties have been shown to vary in an at least approximately linear manner with α – *e.g.* the band gap in SiC (Choyke, Hamilton & Patrick, 1964), and the absorption edge and birefringence in ZnS (Brafman & Steinberger, 1966). Furthermore Brafman, Alexander & Steinberger (1967) have shown that once the constant of proportionality between birefringence ($\Delta\mu$) and percentage hexagonality has been established, equation (2) provides invaluable information for the structure determination of higher polytypes. These authors solved a large number of ZnS polytype structures by using measured birefringence values to restrict the possible Zhdanov symbols to those with a predetermined number of elements, $2k$.

We were not obliged to call upon similar information in order to solve the 'symmetrical' AgI polytypes, but have measured the birefringence of two polytypes 2*H* and 4*H* whose hexagonality is known, and have thereby confirmed the linear dependence of $\Delta\mu$ on α and established the proportionality constant.

Birefringences $\Delta\mu$ were determined by the same method as that described by Brafman & Steinberger (1966) which involves the measurement of optical path difference and crystal thickness. Optical path differences at the wave-length $\lambda=589$ nm were measured by means of a X order Berek rotary compensator. From the poor compensation of Newton's colours obtained in white light (Hartshorne & Stuart, 1970) we infer that the double refraction in AgI is markedly dispersed. The thicknesses of crystal sections were measured by racking down a microscope at magnification 500 × . Accuracy of the results is limited by that of the thickness measurements and is estimated at one or two percent. The mean results from measurements on several specimens are shown in Table 6. Equation (2) can be now re-expressed in the form

$$2k \simeq 56 \,.\, n \,.\, \Delta\mu \,. \qquad (3)$$

Larson & Berman (1934) record a birefringence of 0·01 for iodyrite, the naturally occurring hexagonal AgI. This value is seen to be closer to our result for the $4H$ polytype rather than the $2H$. It is of interest to note that anomalous birefringence is mentioned by Palache, Berman & Frondel (1951) in connexion with iodyrite and miersite (native low-cubic AgI). It is possible therefore that other polytypes will be identified in native AgI.

Table 6. *Measured birefringences $\Delta\mu$ at wavelength $\lambda = 589$ nm for two* AgI *polytypes of known percentage hexagonality α*

Polytype	α	$10^3\,\Delta\mu$
$2H$	100	17·8
$4H$	50	8·9

Summary

AgI has been shown to form polytypic structures other than the low-cubic and hexagonal forms previously reported to occur below 147 °C at atmospheric pressure. Four new polytypes and their layer sequences have been reported here. The predominant structural form of crystals grown by Cochrane's (1967) method is $4H$ (50 % hexagonal) initially. Upon aging at room temperature these crystals appear to transform into higher polytypes with increased hexagonality. The series ends with the formation of the $2H$ (100 % hexagonal) polytype. The $4H \rightarrow 2H$ transformation occurs directly upon heating at ~100 °C. The Zhdanov symbols of polytypes identified to date contain only 1's and 2's, reflecting the absence of extensive cubically packed layer sequences. Birefringences have been measured and the direct proportionality between the percentage hexagonality and degree of birefringence of AgI polytypes has been established.

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