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Lattice Parameters of Zn_3As_2

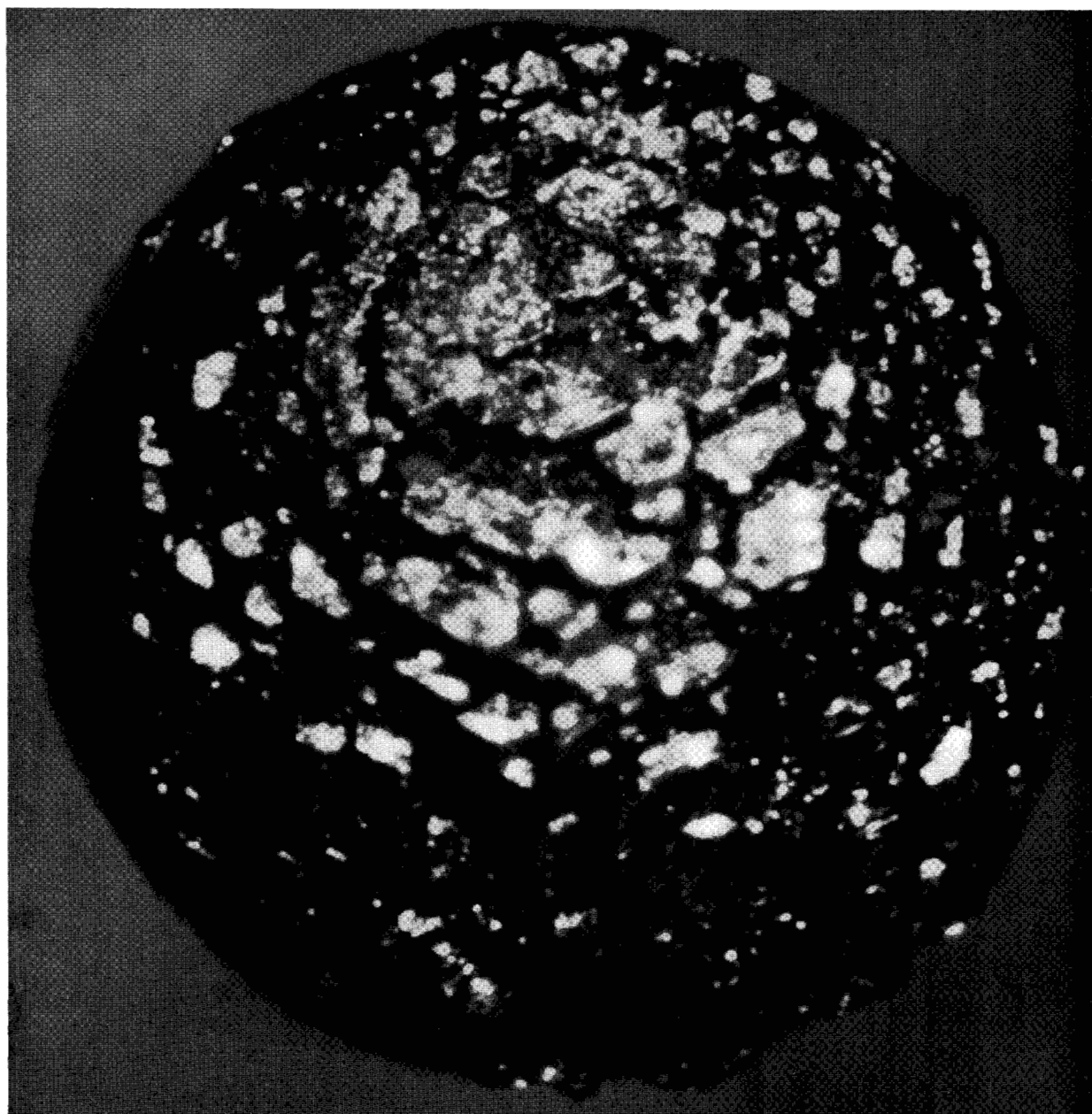


Figure 1

Spherical single crystal of Zn_3As_2 showing growth in preferred directions, which correspond to specific planes in the crystal. Magnification 80X.

Since current research on the intermetallic compound Zn_3As_2 has indicated desirable semiconductor properties, a new determination has been made of its crystal lattice, which had been reported variously as cubic and as tetragonal.

Zn_3As_2 was first reported by Natta and Passerini¹ to have a cubic lattice with cell edge $a = 5.81\text{\AA}$. Later work by Stackelberg and Paulus² showed that the lattice had tetragonal symmetry with $c = 11.45\text{\AA}$ and $a = 8.09\text{\AA}$. The relationship of the two cells was such that the tetragonal cell was twice as high as the cubic and was rotated around the c -axis by 45° with respect to the cubic, the tetragonal a -axes being the face diagonals of the cubic cell. Since most semiconductors have cubic symmetry, the Zn_3As_2 lattice was rechecked at this laboratory in a routine survey. The x-ray spectrometer measurements indicated tetragonal symmetry but with $c = 23.65_2\text{\AA}$ and $a = 11.78_1\text{\AA}$; $c/a = 2.007$. This cell is four times as high as the originally reported cubic cell and is twice as

wide and deep. The strong lines in our patterns are in agreement with the lines reported by Natta and Passerini.

Single crystals of Zn_3As_2 * were grown in a quartz tube by cooling from a melt consisting of the proper mixture of zinc-arsenic compound in order to form Zn_3As_2 . The first sample investigated was an octahedron. Rotation patterns around its three mutually perpendicular axes indicated the spacings reported above. A tetragonal cell was indicated by precession pictures and back-reflection pictures, which showed the necessary fourfold symmetry on the "23.65Å" axis and the necessary twofold symmetry on the other axes. Indexing the patterns in terms of these axes gives a body-centered cell. Other samples gave identical results.

¹G. Natta and L. Passerini, *Gazz. Chem. Ital.*, **58**, 541 (1928).

²M. V. Stackelberg and R. Paulus, *Z. physik. Chem. B* **28**, 427 (1935).

*Prepared at the IBM Research Center, Poughkeepsie, N. Y., by G. Silvey and V. Lyons.

Table 1 Observed reflections from Zn_3As_2 indexed in terms of BC tetragonal lattice

Even values of l								Odd values of l							
hk	$l=0$	$l=2$	$l=4$	$l=6$	$l=8$	$l=10$	$l=12$	hk	$l=1$	$l=3$	$l=5$	$l=7$	$l=9$	$l=11$	$l=13$
00		*	†	*	008	*	0, 0, 12	12	121	123	125	127	129	1, 2, 11	1, 2, 13
11	*	112	*	116	*	1, 1, 10	*	23	231	233	235	237	239	2, 3, 11	2, 3, 13
02	†	†	†	†	†	0, 2, 10	0, 2, 12	14	141	143	145	147	149	1, 4, 11	†
22	†	*	224	*	†	*	2, 2, 12	34	†	343	†	†	349		
13	*	132	†	136	†	1, 3, 10	†	25	†	253	255	257	†	2, 5, 11	2, 5, 13
33	*	332	*	336	*	3, 3, 10	*	45	451	453	455	457	459		
04	040	†	†	†	048	†		16	†	163	165	167	†	†	1, 6, 13
24	†	†	†	246	†	†		36	361	363	365	367	†		
44	440	*	†	*	448	*		56	†	†	†	†	†		
15	*	152	†	156	†			27	271	273	275	277	279	2, 7, 11	2, 7, 13
35	*	352	†	356	†			47	or 181	or 183	†				
55	*	552	*	556	*			67	or 291	or 293	or 295				
06	060	†	064	066				18	or 471	or 473	†				
26	†	†	264	†				38	381	†	†				
46	460	†	†	†				58	581	583	585				
66	660	*	664	*				17	†	†	†				
17	*	172	†												
37	*	372	†												
57	*	572	†												
77	*	772	*												
08	080	†													
28	†	†													
48	480	†													
68	†	†													
88	880	*													

*Forbidden by space group

†Not observed

Reflections also observed: 0, 10, 0; 0, 12, 0; 0, 0, 16; 0, 0, 20; 0, 0, 24

The back-reflection pictures give a Laue symmetry of $4/mmm$. The systematic extinctions indicate that the (001) plane and the forms (100) and (110) are glide planes. The probable space group is then $I4_1/acd - D_{4h}^{20}$. From previous density measurements^{1,2} the number of atoms per cell is 160.

Powder patterns were taken with the G. E. XRD-3 spectrometer but preferred orientation difficulties prevented satisfactory measurements, although the expected lines appeared in the patterns. The lattice parameters were then obtained from spectrometer measurements on

a single crystal with faces cut perpendicular to the (001) and (100) planes. Extrapolation was made to $\theta = 90^\circ$, although no refraction correction was applied. All measurements were made at room temperature. A unique spherical single crystal is shown in Fig. 1.

Table 1 gives a list of reflections observed on precession or rotation photographs. Fig. 2 shows the first few peaks of the powder pattern.

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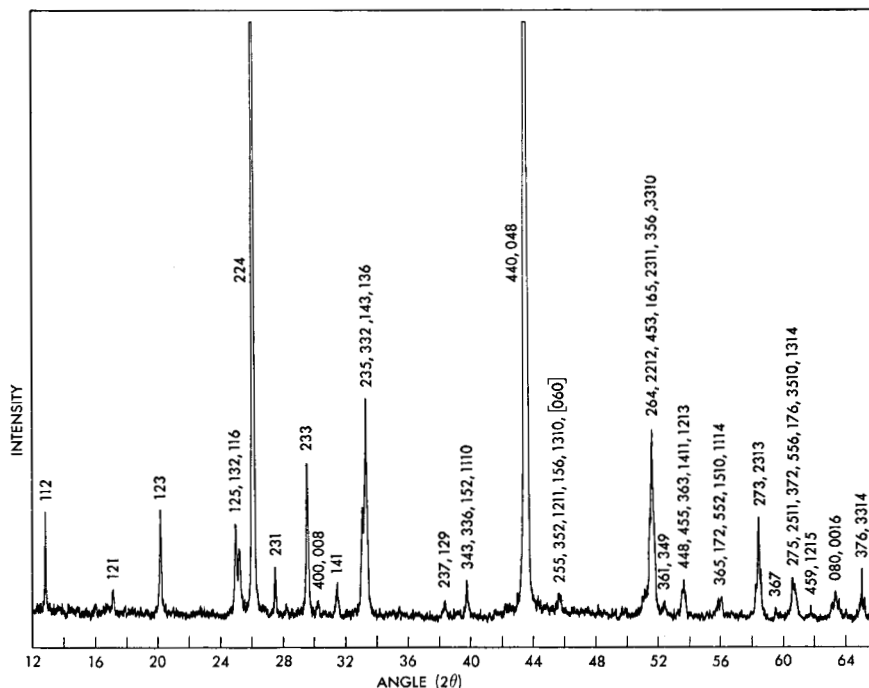


Figure 2
The first few peaks in the powder pattern obtained with Ni-filtered Cu x-radiation and linear recording.