

AN ELECTRON DIFFRACTION STUDY OF THE STRUCTURE OF PbBi_4Te_7

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A full determination of the crystal structure of PbBi_4Te_7 has been carried out. The unit cell: $a = 4.50 \pm 0.02$ A, $c = 17.6 \pm 0.05$ A, space group $D_{3d}^5 - P\bar{3}m1$. The structure is referable to a nine-layer stacking, in which the Pb atoms are distributed statistically in four of the layers together with weights of 3/16 Pb and 13/16 Te. The unit cell contains 3/4 of a formula weight of PbBi_4Te_7 .

Currently, the properties and structure of a great many two-component semiconducting compounds are being studied, and still greater attention is being given to three- and four-component phases, principally those which correspond to pseudobinary compounds.

From this point of view, the systems $\text{SnTe}-\text{Sb}_2\text{Te}_3$ and $\text{PbTe}-\text{Bi}_2\text{Te}_3$ are interesting. Their phase diagrams were studied in [1].

The compound SnSb_2Te_4 is found in the first of these systems. We have determined its structure by electron diffraction methods [2]. In the second system also, according to [1], there exists only one compound, whose composition however is $\text{PbBi}_4\text{Te}_7 = \text{PbTe} \cdot 2\text{Bi}_2\text{Te}_3$. The determination of its structure by electron diffraction techniques is the subject of this paper.

This compound corresponds in composition to an alloy of 82.7% Bi_2Te_3 and 17.3% PbTe .

Measurements showed [1] that the ternary compound PbBi_4Te_7 has an electrical conductivity of about $1700 \text{ ohm}^{-1} \text{ cm}^{-1}$ and a thermo-emf of $31 \mu\text{v/deg}$, and is apparently a semiconducting compound.

The x-ray phase analysis carried out in [1] confirmed the existence of a new phase whose composition may be expressed by the formula PbBi_4Te_7 .

The structures of the "components" of this compound are known. PbTe possesses a structure of the NaCl-type with a cubic unit cell edge of $a = 6.34$ A [3]. Bi_2Te_3 [4] has a rhombohedral structure of the tetradymite type ($\text{Bi}_2\text{Te}_2\text{S}$); the parameters of the hexagonal unit cell are $a = 4.38 \pm 0.01$, $c = 30.4 \pm 0.2$ A.

The samples for electron diffraction study were prepared by the sublimation in a vacuum of a ternary fusion of PbBi_4Te_7 onto a fresh surface of an NaCl crystal. The composition of the resulting film matched the composi-

tion of the initial charge, because the fragment was volatilized completely.

Depending upon the method of annealing the product, the samples investigated gave electron diffraction patterns of three forms which are similar in the position and intensities of their strong reflections, but which differ in their weak reflections.

The unit cells determined from these photographs all appear to be hexagonal; their parameters are

I	$a = 4.50 \pm 0.02$ A,	$c = 17.6 \pm 0.05$ A,
II	$a = 4.44 \pm 0.02$ A,	$c = 71.7 \pm 0.2$ A,
III	$a = 4.44 \pm 0.02$ A,	$c = 107.4 \pm 0.3$ A.

We noted that $c_{\text{II}} \approx 4c_{\text{I}}$, and $c_{\text{III}} \approx 6c_{\text{I}}$. Formally, in view of the differences in the unit cells, it would be proper to regard these three structures as being three different phases of the compound PbBi_4Te_7 .

However, it was further determined that these three phases can be considered as differently ordered forms of one and the same phase; i. e., as superstructures of structure I.

Moreover, a confirmation of this latter view appeared in the electron diffraction photographs of these phases of PbBi_4Te_7 ; that is, their strongest reflections correlate with those ten lines which are observed of x-ray powder photographs of PbBi_4Te_7 . In addition to the data presented in [1], we obtained independently an x-ray photograph of the initial charge, using $\text{FeK}\alpha$ radiation, thus confirming the correspondence.

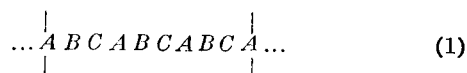
The present article is concerned with the results of the determination of structure I. The sample was obtained by depositing powder on a substrate which was heated to $80-100^\circ\text{C}$, and following this, annealing the whole at a temperature of $\approx 200^\circ\text{C}$ for one hour.

A characteristic electron diffraction pattern of the substance is shown in Fig. 1. Extinctions were observed only on the zero layer line; only those reflections are present which satisfy the condition $h-k=3n$.

The possible space groups here are: $D_{3d}^3 - \bar{P}3m1$, $D_3^2 - P321$, $C_{3i}^1 - \bar{P}3$, and $C_{3v}^1 - P3m1$. The strongest reflections are found on those layer lines with $l=3n$, and for these reflections the rhombohedral condition $h+k-l=0$ holds. From this it follows that the structure is characterized by a pseudoperiod $c'=c/3=5.87 \text{ \AA}$, and within this pseudoperiod the structure appears to be rhombohedral, i. e., it consists of at least three layers; and therefore in the whole true cell there are at least nine layers.

The thickness of a layer appears to be $17.6/9=1.95 \text{ \AA}$. This value agrees excellently with the results of structural studies of other layered semiconductors composed of Te and Bi, which have layer thicknesses of the order of $1.95-2.00 \text{ \AA}$ [5].

Accordingly, proceeding from the conditions of a nine-layer structure in which any of the three successive layers show a rhombohedral symmetry, i. e., implying the presence of cubic packing, the formula of the structure may be symbolized as



It must be emphasized that so far the discussion has been concerned only with the possible geometrical positions of atoms, irrespective of their chemical peculiarities. Otherwise the pseudoperiod would be the true period.

Further analysis was carried out using F^2 - and F -series.

The intensities of the reflections in the electron diffraction patterns obtained from oblique texture photographs were determined microphotometrically and visually [2].

The transformation of intensities to structural amplitudes was carried out according to the formula [6]

$$F_{hkl}^2 = \frac{I_{hkl}}{p d_{hko} d_{hkl}}, \quad (2)$$

where I_{hkl} is the local intensity of the reflection, d is the interplanar spacing, and p is the periodicity factor.

In the first stage, the construction of the F^2 -series, we did not introduce the dynamic correction, which is considered to be principally in the peak heights.

A uniform profile of the F^2 -series along $00z$ (Fig. 2) gave a result which was already evident from the foregoing examination. The peaks in that cross section are situated at a distance of $c/3$ from each other, which confirms the cubic mode of superposition of adjoining layers (1).

Thus, the initial data for the construction of a structure model appeared to be: the geometrical packing formula (1), the possible space groups, and the chemical formula PbBi_4Te_7 . It should be noted that the chemical formula weight, which contains 12 atoms, is found to be in apparent contradiction with a geometrical system of nine layers. Indeed, if we wholly pack one of the layers with Pb atoms, we will not have sufficient room for the eleven remaining atoms. From this it follows that at least some layers must be statistically packed with more than one species of atom. In order to "squeeze" the twelve-atom "formula" into nine layers, we multiply it by $9/12=3/4$, which leads to the "composition" $\text{Pb}_{3/4}\text{Bi}_3\text{Te}_{5\frac{1}{4}}$, and we

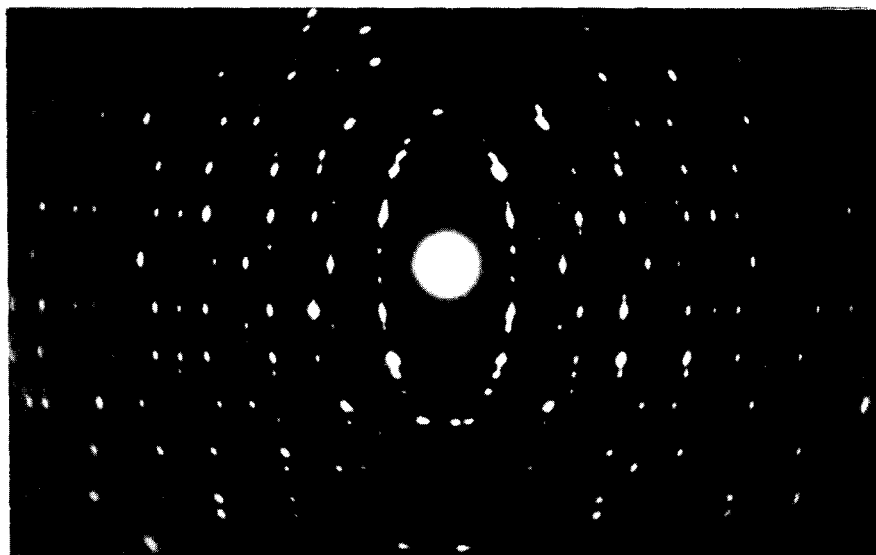


Fig. 1. An oblique texture electron diffraction pattern of PbBi_4Te_7 .

shall investigate the possible variants of this. The simplest of these is to pack three layers with Bi atoms, five with Te atoms, and to dispose $\frac{3}{4}$ Pb and $\frac{1}{4}$ Te statistically in one layer. Also conceivable are variants with a statistical joint disposition of $\frac{3}{4}$ Pb and $1\frac{1}{4}$ Te in two layers, and other schemes such as that. Possible, but less probable, is a statistical distribution of Pb together with Bi, because here, for the complete packing of the layer we must also include Te, i. e., to assume a statistical distribution of three atom species, which is scarcely likely. Consequently, as a first approximation, it is possible to regard the structure as having the composition Bi_3Te_6 , disregarding the fact that $\frac{3}{4}$ Te in such a formula are actually replaced by Pb. At the same time, it is necessary to take into consideration the fact that the contribution of Pb to the structure factor in the analysis of intensities cannot change them very greatly, since the scattering factor of Bi is as great as that of Pb, and that of Te is not much less.

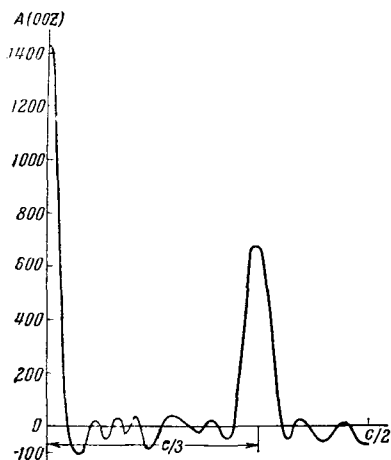


Fig. 2. Uniform profile of the F^2 -series of $A(00z)$.

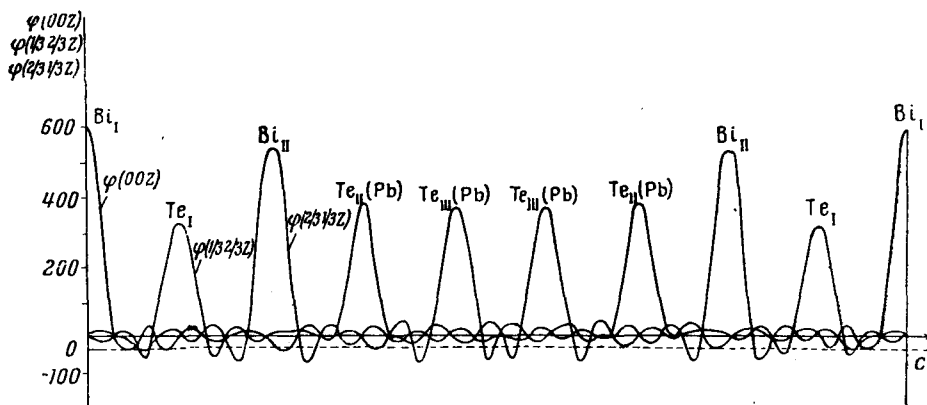
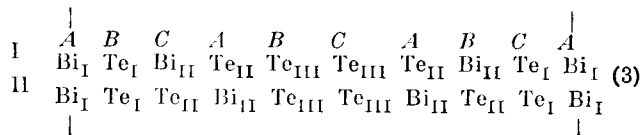


Fig. 3. A combination of the three one-dimensional electron density sections $\varphi(00z)$, $\varphi(\frac{1}{3} \frac{2}{3} z)$ and $\varphi(\frac{2}{3} \frac{1}{3} z)$ (in relative units).

If we assume the natural requirement of an alternation of layers of Bi atoms with layers of Te, for Bi_3Te_6 the following variants of atomic distribution are possible:



These both satisfy the centrosymmetrical space group $D_{3d}^3 - \bar{P}3m1$; the second of these has a true period of $c/3$ and consequently does not satisfy the demands of a nine-layer stratification.

Further analysis was carried out through the comparison of calculated and experimentally observed intensities. The calculation of the intensities of a series of strong and weak reflections showed that variant I produces satisfactory agreement with the observed values, and as a first approximation appears completely acceptable.

The intensities of 180 reflections in the electron diffraction pattern of the structure were measured experimentally. A complicating factor was introduced by the fact that in the majority of cases reflections of the type (hkl) and $(\bar{h}k\bar{l})$ are superimposed to some extent, and their structure factors are not identical in absolute value.

Therefore, the relative contribution of each F from such a pair of structure factors was determined in agreement with their assumed theoretical relationship.

It should be noted that in consequence of this, in later operations—the Fourier syntheses—experimental F_{hkl} 's were introduced again as totals. This procedure did not, however, lessen the clarity of definition of the results.

For the space group $D_{3d}^3 - \bar{P}3m1$, nine atoms $[\frac{3}{4}(\text{Bi}_4\text{Te}_8)]$ may be distributed in the following manner:

- 1 Bi_{II} — in the position 1(a) — 000,
- 2 Te_{II} — in the position 2(c) — 00z, 00 \bar{z} ;
- 2 Te_I } — in the position 2(d) — $\frac{1}{3}, \frac{2}{3}z,$
- 2 Bi_{II} } $\frac{2}{3}, \frac{1}{3}\bar{z}.$
- 2 Te_{III} }

The structure factor has the form

$$\begin{aligned} \Phi_{hkl} = & \frac{1}{2} f_{\text{BiI}} + f_{\text{TeII}} \cos 2\pi \frac{l}{3} \\ & + f_{\text{TeI}} \left[\cos \pi i \cos \pi \left(\frac{k-h}{3} + \frac{2l}{9} \right) \right] \\ & + f_{\text{BiII}} \left[\cos \pi i \cos \pi \left(\frac{h-k}{3} + \frac{4l}{9} \right) \right] \\ & + f_{\text{TeIII}} \left[\cos \pi i \cos \pi \left(\frac{k-h}{3} + \frac{8l}{9} \right) \right]. \end{aligned} \quad (4)$$

An analysis of the electron diffraction patterns indicated that the intensities depart observably from the cinematographic law of dispersion. Therefore we introduced a dynamic correction according to the method used in (7), taking the thickness of the crystals as 320 Å.

After the introduction of the dynamic correction, the divergence factor diminished from 40 to 27%. At that stage it became necessary to take into account the scattering by the Pb atoms, which had been previously neglected. The most natural approach seemed to be place $\frac{3}{4}$ of the Pb atoms together with the Te_{III} atoms; this separated four successive layers of Te atoms by two layers consisting statistically of $1\frac{1}{4}$ Te and $\frac{3}{4}$ Pb atoms. In that case, the scattering factor of Te_{III} in (4) is replaced by $\frac{1}{2}(\frac{3}{4}f_{\text{Pb}} + 1\frac{1}{4}f_{\text{Te}}) = \frac{3}{8}f_{\text{Pb}} + \frac{5}{8}f_{\text{Te}}$. This hypothesis improved the convergence, but, as is seen below, did not prove to be completely correct. Determining the signs of the amplitudes, we constructed a one-dimensional sections of the three-dimensional series $\varphi(00z)$ and $\varphi(\frac{1}{3}\frac{2}{3}z)$ (Fig. 3). It is not difficult to see from (3) that in the first of these atoms A: Bi_I and Te_{II} are located, and in the second, atoms B: Te_I and Te_{III}; the section $\varphi(\frac{2}{3}\frac{1}{3}z)$ places the C atoms, which are inversely equal to the B atoms. The combination of all three sections is shown in Fig. 3.

The peak heights in the sections of Fig. 3 at once indicated to us the accuracy of the model which we had postulated, but also revealed the inaccuracy of it in regards to the disposition of the Pb atoms; the peaks for Te_{II} and Te_{III} appeared to have equal height, both greater than the peak for Te_I. This indicates that $\frac{3}{4}$ Pb is placed together with the Te not only in position III, but in position II as well.

Calculating the intensities for this arrangement involves equating the scattering factor for positions II and III: $\frac{1}{4}(3\frac{1}{4}f_{\text{Te}} + \frac{3}{4}f_{\text{Pb}}) = \frac{13}{4}f_{\text{Te}} + \frac{3}{16}f_{\text{Pb}}$. Such a calculation resulted in a reduction in the reliability coefficient to 23.6%. The values of F_{obs} and F_{calc} are given in the table. Consequently, the Pb and Te atoms are distributed statistically in the layers with the weights mentioned. Since the signs of the structure factors did not change, the synthesis of Fig. 3 appears to be final.

Therefore, formula (3) must be rewritten in the following form:

$$\begin{array}{c} | \\ A_1 \quad B_1 \quad C_1 \quad A_2 \quad B_2 \quad C_2 \quad A_3 \quad B_3 \quad C_3 \quad A_1 \dots \\ \text{Bi}_I \quad \text{Te}_I \quad \text{Bi}_{II} (\text{Te}_{\frac{13}{16}} \quad \text{Pb}_{\frac{3}{16}})_{II} \quad (\text{Te}_{\frac{13}{16}} \quad \text{Pb}_{\frac{3}{16}})_{III} \quad (\text{Te}_{\frac{13}{16}} \quad \text{Pb}_{\frac{3}{16}})_{III} \quad (\text{Te}_{\frac{13}{16}} \quad \text{Pb}_{\frac{3}{16}})_{II} \quad \text{Bi}_{II} \quad \text{Te}_I \quad \text{Bi}_I \dots \\ | \end{array} \quad (5)$$

This packing of atoms is shown in Fig. 4.

The z coordinates of the peaks agree almost exactly with the ideal positions $\frac{1}{9}, \frac{2}{9}, \frac{3}{9}, \dots$. These coordinates are as follows: $z_{\text{TeI}} = 0.110, z_{\text{TeII(Pb)}} = 0.333, z_{\text{TeIII(Pb)}} = 0.444, z_{\text{BiII}} = 0.778$.

An estimate of the contribution of Pb to peaks II and III could be accomplished as well on the basis of the peak heights. In addition to this, in view of the possible influence of any inaccuracy in the dynamic correction to the peak heights, we proceeded not from theoretical appraisals of these heights, but from the experimental observations.

The Fourier syntheses (Fig. 3) were constructed without the zero term F_{000} . Its contribution may be estimated as being approximately equal to the mean negative value of the potential in the syntheses [6, 8]. Therefore we began by reading the heights of the peaks from the dashed line in Fig. 3. Taking into consideration the fact that the scattering factors of the Bi and Pb atoms are practically identical, we took the mean of the heights of the Bi_I and Bi_{II} maxima as the peak height for the Pb atom. The height of the Te_I peak is equivalent to the height of the pure Te atom.

Proceeding from these heights and the heights of four mean Te_{II(Pb)} and Te_{III(Pb)} peaks, it was readily possible to determine that they correspond to a content of 17% Pb for example, which agrees satisfactorily with the ideally calculated quantity of lead, $\frac{3}{16} = 18.7\%$.

The close agreement of these values confirms the conclusion that the atoms are distributed in accordance with formula (5).

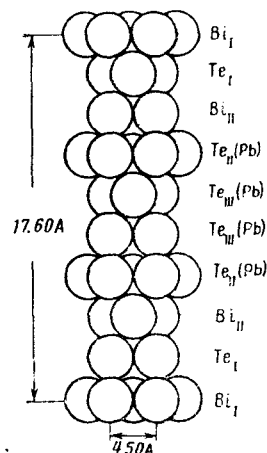


Fig. 4. The packing of the atoms in the unit cell of PbBi₄Te₇.

A Comparison of the Calculated and Experimentally Observed* Structural Amplitudes

hkl	Φ_c	$ \Phi_e $	hkl	Φ_c	$ \Phi_e $	hkl	Φ_c	$ \Phi_e $
101	+3.34	1.97	20.11	+0.98	1.75	30.13	+1.23	2.36
$\bar{1}01$	-0.87	0.68	$\bar{2}0.11$	+1.73	2.12	30.14	+1.24	2.30
102	+3.36	1.92	20.12	+14.75	11.67	30.18	+8.73	5.84
$\bar{1}02$	+1.24	0.72	$\bar{2}0.12$	-0.22	0.22	30.19	+0.88	1.48
103	+0.23	0.23	20.13	+2.41	3.30	220	+14.22	12.54
$\bar{1}03$	+36.99	29.8	$\bar{2}0.13$	-1.32	1.82	224	+1.64	2.24
104	-0.98	1.1	20.15	-0.18	0.18	225	+0.64	0.97
$\bar{1}04$	+1.11	1.85	$\bar{2}0.15$	+12.45	10.24	229	+11.91	9.80
105	+1.01	1.00	20.16	+2.88	3.91	22.10	+1.33	2.42
$\bar{1}05$	-0.73	0.47	$\bar{2}0.16$	+1.35	1.12	22.13	+1.18	1.82
106	+29.65	29.4	20.17	+1.25	3.40	22.14	+1.10	1.88
$\bar{1}06$	-0.37	0.37	$\bar{2}0.17$	-2.11	2.36	22.15	-0.65	0.88
107	+0.87	1.90	20.18	-0.67	1.14	22.18	+8.20	6.46
$\bar{1}07$	+2.32	3.09	$\bar{2}0.18$	-0.17	0.17	22.19	+0.83	1.20
108	-0.61	0.81	20.19	-0.60	0.81	311	-0.41	0.47
$\bar{1}08$	+2.27	2.95	$\bar{2}0.19$	+1.17	1.63	131	+1.45	1.56
10.10	+2.00	3.06	211	+2.03	1.72	312	+0.33	0.97
$\bar{1}0.10$	-0.54	0.48	121	-0.21	0.54	132	+1.38	1.76
110	+28.80	30.40	212	+1.93	1.64	313	+13.32	10.45
111	+0.88	0.97	122	+0.53	0.97	133	-0.19	0.19
114	+2.27	2.65	213	-0.25	0.25	314	+1.40	1.79
115	+2.26	2.56	123	+18.59	16.2	134	-0.48	0.96
116	+0.17	0.24	214	-1.13	1.57	315	-0.61	0.82
118	+0.73	1.04	124	+0.88	1.54	135	+1.38	1.46
119	+19.14	20.5	215	+1.88	2.54	316	-0.18	0.18
11.10	+1.65	2.90	125	-0.64	0.89	136	+12.44	10.75
11.13	+1.50	3.14	216	+17.06	15.56	317	+1.31	2.34
11.14	+1.46	2.51	126	-0.24	0.24	137	+1.35	1.86
11.15	-1.18	2.31	217	+1.45	1.88	318	+1.31	2.31
11.18	+10.69	8.31	127	+1.72	3.36	138	-0.81	0.71
201	-0.47	0.58	218	-0.42	0.58	31.10	-0.61	0.82
$\bar{2}01$	+2.51	1.95	128	+1.66	2.42	13.10	+1.25	1.67
202	+1.68	1.43	219	-0.22	0.95	31.11	+0.93	1.23
$\bar{2}02$	+2.48	1.44	129	-0.22	0.22	13.11	+1.24	1.98
203	+24.07	23.7	21.10	-0.81	0.89	31.12	+10.14	8.35
$\bar{2}03$	-0.34	0.34	12.10	+0.38	1.06	13.12	-0.16	0.16
204	+1.67	1.65	21.11	+1.45	1.93	31.13	+1.32	1.56
$\bar{2}04$	-0.60	0.93	12.11	+0.38	1.06	13.13	-0.98	1.43
205	-0.48	0.66	21.12	-0.19	0.19	31.15	-0.43	0.43
$\bar{2}05$	+0.68	1.20	12.12	+13.00	9.8	13.15	+8.96	7.63
206	-0.31	0.31	21.13	-1.09	1.86	31.16	+1.90	1.74
$\bar{2}06$	+21.09	18.94	12.13	+2.36	3.52	13.16	+0.85	1.10
207	+2.21	3.74	21.15	+11.14	9.46	401	+1.31	1.73
$\bar{2}07$	+1.68	2.10	12.15	-0.17	0.17	$\bar{4}01$	-0.89	0.52
208	+2.00	3.38	21.16	+1.32	2.04	402	-1.31	2.26
$\bar{2}08$	-0.87	1.17	12.16	+1.25	2.70	$\bar{4}02$	+0.88	1.23
209	-0.86	1.42	21.17	-0.99	0.72	403	-0.18	0.18
$\bar{2}09$	-0.26	0.26	12.17	+1.18	2.38	$\bar{4}03$	+11.68	9.65
20.10	-0.84	1.10	21.18	-0.44	0.60	404	-1.09	1.51
$\bar{2}0.10$	+1.89	2.66	12.18	-0.14	0.14	$\bar{4}04$	+2.33	2.86
			21.19	+1.04	2.13	406	+11.14	9.00
			12.19	-0.70	0.95	$\bar{4}06$	-0.17	0.17
			300	+16.84	14.24	407	+0.98	1.28
			304	+1.75	3.19	$\bar{4}07$	+1.27	1.52
			305	+1.66	2.98	408	-0.80	0.98
			308	+0.40	1.02	$\bar{4}08$	+1.24	1.85
			309	+13.66	11.32	40.10	+2.42	3.70
			30.10	+1.59	2.40	$\bar{4}0.10$	-0.91	1.02

* Dynamic correction included.

TABLE (Continued)

hkl	Φ_c	$ \Phi_e $	hkl	Φ_c	$ \Phi_e $	hkl	Φ_c	$ \Phi_e $
40.11	+1.03	1.44	414	+1.10	1.34	513	-0.11	0.11
40.11	+0.88	1.12	415	+1.02	1.36	153	+7.42	5.84
40.12	-0.13	0.13	418	+1.29	1.52	516	+7.30	5.94
40.12	+9.27	7.57	419	+7.73	5.85	156	-0.12	0.12
40.13	-1.47	2.20	41.10	+0.86	1.04	517	+0.84	1.08
40.13	+0.86	1.95	41.13	+0.96	1.51	157	+0.99	1.11
40.15	+8.29	6.33	41.14	+0.89	1.09	51.10	+1.82	1.54
40.15	-0.13	0.13	41.18	+5.74	4.70	15.10	-0.78	1.01
40.16	+2.04	2.30	503	+8.55	6.15	51.11	+0.88	1.13
40.16	+2.29	3.10	503	-0.13	0.13	15.11	+0.92	1.21
40.17	-1.08	1.40	506	-0.13	0.13	51.12	-0.11	0.11
40.17	+2.85	3.53	506	+8.29	6.35	15.12	+6.52	4.91
40.18	-0.98	1.16	507	+0.96	1.16	51.15	+5.97	4.41
40.18	-0.12	0.12	507	+0.96	1.16	15.15	-0.10	0.10
40.19	+0.89	1.10	508	+0.89	1.12	51.16	+0.81	0.93
40.19	-0.68	0.95	508	-0.98	1.21	16.16	+1.69	2.54
321	+1.24	2.60	50.10	-0.90	1.30	600	+6.84	5.25
231	+0.74	1.06	50.10	+0.96	1.13	609	+6.11	5.60
322	+1.24	2.14	50.12	+6.30	5.10	60.10	+0.87	1.09
232	+0.92	1.15	50.12	-0.12	0.12	431	+0.83	1.03
323	-0.16	0.16	50.16	+0.88	1.18	341	-0.38	0.59
233	+10.37	8.28	50.16	+6.84	6.84	433	-0.11	0.11
324	-0.60	0.68	330	+8.29	6.68	343	+6.52	5.12
234	+0.92	1.13	334	+0.96	1.15	436	+6.42	5.12
326	+8.82	7.92	335	+0.89	1.04	346	-0.10	0.10
236	-0.14	0.14	339	+6.52	5.27	437	+0.60	0.96
327	+0.98	1.11	33.10	+0.24	0.85	347	+1.75	2.45
237	+1.17	1.52	421	-0.37	0.68	43.12	-0.09	0.09
328	-0.69	0.60	241	+0.96	1.14	34.12	+5.75	4.38
238	+1.09	1.97	423	+7.96	6.50	43.15	+5.44	3.92
32.10	+0.97	1.14	243	-0.12	0.12	34.15	-0.10	0.10
23.10	-0.68	0.86	426	-0.11	0.11	43.16	+0.98	1.73
32.11	+0.97	1.12	246	+7.74	6.20	34.16	+0.89	1.62
23.11	+0.87	1.03	427	+0.89	1.15	520	+6.52	5.63
32.12	-0.12	0.12	247	+0.88	1.22	524	+0.75	1.49
23.12	+8.42	7.58	428	+0.82	1.01	529	+4.88	4.10
32.13	-1.06	1.66	248	-0.97	0.89	52.10	+0.84	1.45
23.13	+0.84	1.00	42.10	-0.58	0.77	52.13	+1.68	2.57
32.15	+6.74	5.85	24.10	+0.89	1.18	613	+5.98	4.73
23.15	-0.11	0.11	42.11	+1.73	2.64	163	-0.10	0.10
32.16	+0.89	1.09	24.11	+0.82	1.12	616	-0.09	0.09
23.16	+0.82	1.16	42.12	+5.84	4.87	166	+5.75	4.48
410	+9.89	8.10	24.12	-0.12	0.12	61.12	+5.12	5.12
411	+0.94	1.11	42.15	-0.10	0.10	16.12	-0.08	0.08
			24.15	+5.43	4.90	61.15	-0.08	0.08
						16.15	+4.88	3.28
						440	+5.65	4.15

The shortest interatomic distances (between layers) in the structure are as follows:

$$\text{Bi}_I - \text{Te}_I = 3.24 \text{ \AA},$$

$$\text{Bi}_{II} - \text{Te}_{II} (\text{Pb}) = 3.25 \text{ \AA},$$

$$\text{Te}_I - \text{Bi}_{II} = 3.26 \text{ \AA},$$

$$\text{Te}_{II} (\text{Pb}) - \text{Te}_{III} (\text{Pb}) = 3.24 \text{ \AA}.$$

The distances within a layer are equal to the a period of the unit cell, viz 4.50 Å. Apparently, their proximity is explained by the statistical packing of positions Te_{II} and Te_{III} .

The structural analysis proved that there is no reason for writing the chemical formula of the compound PbBi_4Te_7 as $\text{PbTe} \cdot \text{Bi}_2\text{Te}_3$, since in its structure there are no domains of "initial" structures as such; however, a great many of their characteristic lines do persist in the pattern of the compound.

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All abbreviations of periodicals in the above bibliography are letter-by-letter transliterations of the abbreviations as given in the original Russian journal. *Some or all of this periodical literature may well be available in English translation.* A complete list of the cover-to-cover English translations appears at the back of this issue.
