It may be assumed that the elongations observed correspond to plate formation in the solid-solution matrix, in which case we estimate these regions to be about 40 Å across and four atomic layers thick.

The structural changes in the Cu–5 at.% Al crystal are shown by the way in which the intensities are redistributed: the maximum intensity in the central part of the 020 reflexion increases to 120 per unit value and that of $\bar{1}11$ decreases to 60 per unit value. The intensity change may be attributed to the formation of Al atom clusters which distort the regularity of the matrix (Cu atoms are appreciably smaller than Al atoms). This causes distortions which, in their turn, change intensities.

A further increase in the alloying-element concentration leads to a change in the diffuse intensity distribution. The shapes of isointensity curves for Cu alloyed with 10 and 14 at.% Al are shown in Fig. 2(*d*) and (*e*) respectively. Between the $\bar{1}11$ and 020 sites there are elongations of weak intensity. Measurement between the $\bar{1}11$ and 020 sites as a function of scattering angle (or displacement vector **g**) shows that the intensity drops in proportion to $1/g$ (a log plot, Fig. 3), as expected for large distortions (Krivoglaz, 1967). It is therefore reasonable to expect that an increase in the alloying-element concentration would be accompanied by appreciable distortions in the solid-solution lattice.

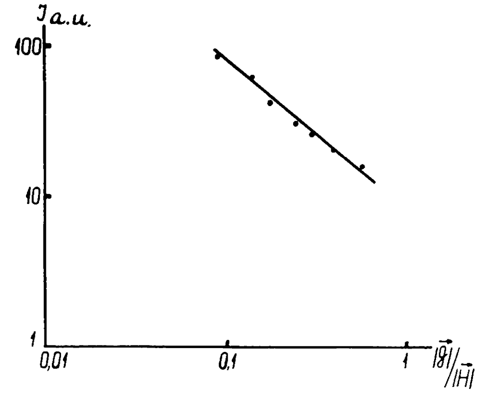

Fig. 3. Dependence of diffuse scattering intensity on displacement wavevector |**g**|.

These distortions might be associated with the formation of atom conglomerations within the solid-solution structure which lose coherence with the matrix lattice. This is supported by separation of sites $\bar{1}11$ and 020 (Fig. 2*d*,*e*).

In addition, the X-ray pictures of Cu–10 and 14 at.% Al display new diffuse reflexions which are absent at lower Al concentrations. As seen in Fig. 1, the six diffuse reflexions observed are near the primary beam at the vertices of a perfect hexagon whose sides are formed by the diffuse background in the shape of hyperbolae pointing towards the primary beam. The intensity of the six spots is roughly similar to that of the four diffuse reflexions considered earlier.

It is difficult to propose an unambiguous interpretation of the new diffuse reflexions. They may arise from the new configurations of Al atoms about Cu atoms. A configuration was considered (Epperson, Fürurohr & Ortiz, 1978) in which four Al atoms occupy a tetrahedron centred on the Cu atom with four Al atoms at the vertices. This corresponds to the trigonal symmetry of the six diffuse reflexions. It may be assumed that the new reflexions together with the $\bar{1}11$, 020 reflexions' separation indicate that the new regions appear. At growing concentrations these regions become nucleation centres for the new α_2 phase.

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Comments on *The rigid-body vibrations of molecules in crystals* by Burns, Ferrier & McMullan (1967).

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Abstract

The rigid-body analysis of the thermal vibrations in seventeen molecular structures by Burns, Ferrier & McMullan [*Acta Cryst.* (1967), **22**, 623–629] has been repeated and major discrepancies have been observed. The sources of errors have been diagnosed and the relevant comments together with the new list of results are reported.

The criterion put forward by Burns *et al.* (1967) (BFM1) for the verification of the assumed rigid-body motion of molecules has been used by various authors in their work

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(Caron, Riche, Pascard-Billy & Gramain, 1977; Caron, Pascard, Agami & Kasakos, 1978; Brisse & Perez, 1976; Nimmo & Lucas, 1976) and has also been cited in text books (*e.g.* Willis & Pryor, 1975). A recalculation of these criterion parameters for the seventeen example molecules given in BFM1 necessitated the reporting of various oversights and corrections encountered. Only a minor part of one of these oversights for one of the examples (No. 3 in BFM1) was mentioned by the same authors in their later work (Burns, Ferrier & McMullan, 1968) (BFM2) but the others have remained unnoticed up to this date. Although this work in no way alters the notion of the criterion parameters, the correction of the results is obviously necessary for such a basic reference paper for authors wishing to utilize it.

The computer program *TERRIG* (Armağan & Yücel, 1982), written for the calculation of the Burns criterion parameters using the **TL** technique of Cruickshank (1956), was employed throughout the work.

Identical results to those of BFM1 were obtained by performing the calculations with the inclusion of the errors. Errors in the individual examples are summarized in Table 1 and the new list of results are presented in Table 2. The major change observed is the shift of example 9 from the doubtful group to the rigid group.

The authors wish to thank Mrs M. D. Yücel for her help in the computer calculations.

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Table 1. *Brief comments on errors and their consequences*

Notation used is the same as in BFM1.

Example no.	Remarks
1	A misprint. Sign of the size parameter of O(3) should be minus.
3	In the temperature factor, 2 has been omitted for $b_{ij}(i \neq j)$. The comparison parameters of BFM1 could not be accounted for.
4	Omission of the factor 2 for $b_{ij}(i \neq j)$ responsible for all the discrepancies.
5–6	In addition to the error made in example 4, b_{13} mistakenly interchanged with b_{23}.
7	A probable mishandling of the b_{ij}s of C(5) causing variations up to $0\cdot8\ \sigma(U^o)$ in the size parameters.
8	Molecule is *not* centrosymmetric as stated in BFM2. Variations in U^o reaching up to $0\cdot5\sigma$.
9	Calculations have been mistakenly carried out on only half of the molecule. It must be classified almost unequivocally as rigid.
10	U^os of C(1) and C(10) should be $0\cdot1689$ and $0\cdot1593$ Å^2, respectively. Probable misprints.
11	A probable unit-cell parameter mishandling. U^os of BFM1 systematically larger than ours, difference reaching up to $0\cdot8\sigma$.
13–14	$b_{ij}(i \neq j)$ mistakenly *divided* by 2. The resulting discrepancy in U^os reaching up to 2σ.
15	A misprint. C(3) should have been N(3).
17	A probable mishandling of the thermal parameters of C(11) causing a discrepancy of $0\cdot8\sigma$ in U^o.

Table 2. *Revised size, shape and orientation parameters for thermal ellipsoids in eleven of the seventeen molecular structures where major corrections have occurred*

	U^o (Å^2 ×10^4)	U^o-U^c (Å^2 ×10^4)	(σ)	S	θ (°)	
Example 3						
C(1)	1555	−56	(89)	181	8	R
C(2)	1535	−51	(89)	39	12	R
C(3)	1381	−30	(89)	18	13	R
C(4)	1809	83	(89)	81	12	R
C(5)	2155	26	(89)	9	13	R
C(6)	2000	−14	(89)	39	16	R
C(7)	2111	139	(89)	26	15	R
C(8)	1785	−14	(89)	1	7	R
C(9)	1554	−199	(89)	6	11	R
C(10)	2014	81	(89)	51	8	R
C(11)	2194	17	(89)	14	12	R
C(12)	2255	27	(89)	12	23	R
C(13)	2096	71	(89)	98	23	R (1,2)
C(14)	1758	−44	(89)	3	17	R
Example 4						
C(1)	1100	−43	(28)	10	9	R
C(2)	1417	48	(31)	1	14	R
C(3)	1563	10	(33)	10	16	R
C(4)	1606	−1	(36)	21	4	R
C(5)	1521	−50	(36)	3	8	R
C(6)	1419	38	(32)	6	3	R
Example 5						
O(1)	1048	−93	(43)	79	5	?
C(1)	766	18	(43)	33	12	R
C(2)	861	50	(43)	52	7	R
C(3)	806	17	(43)	52	11	R
Example 6						
O(2)	1036	−67	(43)	50	3	R
C(4)	829	55	(43)	7	12	R
C(5)	878	25	(43)	24	3	R
C(6)	820	−13	(43)	6	12	R
Example 7						
C(1)	1226	−20	(65)	3	35	NR
C(2)	1508	−23	(71)	29	8	R
C(3)	1543	−25	(73)	51	9	R
C(4)	1402	43	(68)	15	21	R
C(5)	1367	17	(68)	63	15	R
C(6)	1580	37	(78)	18	12	R
C(7)	1482	−28	(76)	11	10	R
Example 8						
C(1)	1781	1	(44)	80	34	NR
C(2)	2135	−65	(69)	33	20	R
C(3)	2660	39	(77)	8	26	?
N(4)	2277	26	(62)	177	22	?
O(5)	2800	−2	(63)	22	29	NR (1,2)
Example 9						
C(1)	1878	−44	(43)	17	12	R
C(2)	1695	−10	(38)	20	5	R
C(3)	1863	29	(43)	13	17	R
C(4)	1861	49	(44)	3	29	?
C(5)	1720	−9	(41)	24	18	R
C(6)	1842	9	(44)	21	7	R
C(7)	1819	39	(43)	39	37	NR
C(8)	1879	−63	(46)	4	24	R (2,3)
Example 11						
N(1)	999	−57	(36)	4	15	R
C(2)	922	−46	(37)	48	26	?
N(3)	978	9	(35)	184	13	?
C(4)	837	−30	(35)	85	34	R (2,3)
C(5)	874	61	(35)	40	21	R
C(6)	1068	59	(40)	78	27	?
O(7)	1280	49	(37)	267	22	NR
N(8)	1179	−40	(40)	79	5	R
C(9)	1021	57	(41)	1	15	R
C(10)	916	−88	(36)	206	32	NR
O(11)	1127	−18	(30)	460	28	NR (1,2)
O(12)	1325	45	(35)	14	37	NR
Example 13						
N(1)	1663	140	(14)	132	24	NR (2,3)
C(2)	1391	5	(16)	94	26	?
N(3)	1304	−55	(11)	92	23	NR (2,3)
C(4)	1326	−51	(12)	57	10	NR
C(5)	1675	101	(16)	12	31	NR
C(6)	1803	122	(18)	81	24	NR
N(7)	1912	−75	(16)	179	3	NR
O(8)	1698	−186	(11)	185	10	NR
Example 14						
N(1)	1555	88	(12)	30	31	NR
C(2)	1313	−86	(12)	36	18	NR
N(3)	1307	−15	(10)	103	19	R
C(4)	1393	9	(14)	197	49	NR (2,3)
C(5)	1625	61	(15)	79	28	NR
C(6)	1647	103	(15)	86	46	NR
N(7)	1848	−145	(15)	105	36	NR
O(8)	1780	−16	(10)	23	17	R
Example 17						
O(1)	1510	−108	(89)	407	10	NR
O(2)	1965	113	(89)	46	42	NR
C(3)	1232	59	(116)	309	56	NR (1,2)
C(4)	965	−311	(116)	1259	30	NR
C(5)	1096	−259	(116)	1242	37	NR (1,2)
C(6)	765	−197	(116)	2441	38	NR (1,3,2)
C(7)	983	4	(116)	347	46	NR (1,2)
C(8)	1301	70	(116)	605	28	NR (2,3)
C(9)	1689	102	(116)	160	24	? (1,2)
C(10)	2049	430	(116)	672	30	NR (1,2)
C(11)	1772	82	(116)	46	47	NR
C(12)	1521	15	(116)	447	51	NR

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Radii of gyration and scattering curves of hollow bodies of homogeneous electron density: errata.

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Abstract

Equations (15), (16), (17), (18), and (20) in the paper by Hiragi & Ihara [*Acta Cryst.* (1981), A**37**, 378–382] are incorrect. These equations should be as follows:

$$F = 4A^2 C \left[\sum_{k=1}^{n} f\left(s_1, \varphi - \frac{2\pi}{n} k\right) \right] \Psi_C, \tag{15}$$

$$\begin{aligned} f(s_1, \beta) = {} & \left[s_1^2 A^2 \left(\tan^2 \frac{\pi}{n} \sin^2 \beta - \cos^2 \beta \right) \right]^{-1} \\ & \times \left\{ \exp(i s_1 A \cos \beta) \right. \\ & \times \left[i \cot \beta \sin\left(s_1 A \tan \frac{\pi}{n} \sin \beta \right) \right. \\ & \left. \left. - \tan \frac{\pi}{n} \cos\left(s_1 A \tan \frac{\pi}{n} \sin \beta \right) \right] + \tan \frac{\pi}{n} \right\}, \end{aligned} \tag{16}$$

$$V = 2\pi ABC, \tag{17}$$

$$F = \frac{4\pi ABC J_1(s_1, K)}{s_1 K} \Psi_C, \tag{18}$$

$$F = 4\pi ABC \frac{\sin(sL) - sL \cos(sL)}{(sL)^3}. \tag{20}$$

Equations (15) and (16) in the original article lead to incorrect scattering intensity, whereas equations (17), (18), and (20) give the correct but unnormalized value. The figures in the article were calculated with the correct equations and hence need no alteration.

All information is given in the *Abstract*. The authors thank Dr P. Martel for pointing out the errors.

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Commission on Journals

Decisions taken at meetings in Ottawa, August 1981

The attention of authors planning to submit papers to *Acta Crystallographica* or *Journal of Applied Crystallography* is drawn to the following decisions taken by the Commission on Journals at meetings held in Ottawa, 14–16 August 1981. These and other revisions in editorial policy since 1978 will be published in a new version of *Notes for Authors*, which is presently in preparation.

International Symbols for Units

The Commission has recognized that, although multiples of 10^3 are the preferred prefixes in the SI System of Units, the centimetre is not prohibited by the SI system and therefore density and absorption coefficients may be given in units of g cm^{-3} and cm^{-1} respectively, if authors so wish. In all other cases, however, authors are asked to use the recommended prefixes of decimal multiples and submultiples of the SI units rather than using '$\times 10^n$'.

Structural Papers

Estimated standard deviations for B_{eq}. The requirement of estimated standard deviations on equivalent values of the