12-Amorphous, Imperfectly Ordered and Quasi-periodic Materials

PS-12.01.31 INDEXING OF X-RAY POWDER DIFFRACTOGRAMS OF PHASES WITH GIANT UNIT-CELLS WITH THE AID OF ELECTRON DIFFRACTION PATTERNS. By X.L. Ma* and K.H. Kuo, Beijing Laboratory of Electron Microscopy, Chinese Academy of Sciences, P.O. Box 2724, Beijing, China; Department of Material Engineering, Dalian University of Science and Technology, Dalian 116023, China

A new modification of the monoclinic $Al_{13}Co_4$ with rather large lattice parameters (a=3.984, b=0.8148, c=3.223 nm, β=107.97°) has been found. Being an approximant of the decagonal quasicrystal with a giant unit-cell, many reflections sometimes occur very close to each other in certain angle ranges. Trials to index this diffractogram by computer-aided programs all failed. On the other hand, indexing the electron diffraction patterns of important zone axes present no difficulty at all, but only rather inaccurate lattice parameters can be obtained. Using very thin specimens so that the dynamical diffraction effect can be kept low, strong spots in these patterns can be singled out. They should also appear in the X-ray powder diffractogram. With these reflections, about 40% of the observed ones, properly indexed, there was no difficulty to index the complete diffractogram and to calculate the accurate lattice parameters given above. This method has been successfully used in indexing of X-ray powder diffractograms of a number of intermetallic phases with giant unit cells.

PS-12.01.32 THE INCOMMENSURATE STRUCTURE FEATURE OF γ– ALUMINA By Hao Jianmin*, Zhang Shimin, Tianjin Electronic Material Research Institute P.O. Box 55, Tianjin, 300192 and Chen Jizhou, Tianjin Technology Institute, Tianjin 300191, China.

A typical XRD pattern exhibits normal reflection broadening as a function of 2θ scanning angle in a smooth manner. It has been explained that small crystal size, microstress and stacking faults can make the diffraction peaks broaden anomalously. (Author, Klug H.P. et. X–Ray Diffraction Procedures, 1974. D.A.Mirzayen, et.Phys. Met.Metall.1987,64,89–100) The XRD powder patterns of γ– alumina exhibit another anomalous reflection broadening in two aspects: (a) irregular broadening among peaks of different hkl's (even from the same crystal zone), (b) the formation of an odd peak shape with broadened base and sharp top. It has been proposed that γ– alumina has a defect spinel structure. (Author, Rong–sheng Zhou, et. Acta Cryst. 1991, B47, 617–630)

In this paper, an expression of XRD integrated width to the different coherent domain sizes associated with sublattices is given. Let the coherent domain sizes of tetrahedral and octahedral aluminum and the oxygen sublattice be L_3, L_2 and L_1 respectively, the diffraction integrated width β can be written as:

$$\beta = \frac{A^2 + n_1B^2 + n_2C^2 + 2n_1n_2BC + 2n_1AB + 2n_2AC}{(A^2 + 2n_1AB + 2n_2AC)L_1 + (n_1B^2 + 2n_1n_2BC)L_2 + n_2C^2L_3} \cdot \frac{\lambda}{\cos\theta}$$

where: $A = a_Af_A$, $B = a_Bf_B$, $C = a_Cf_C$. A,B,C are the structure factors of the oxygen, the octahedral and tetrahedral aluminum sublattices respectively. n_1, n_2 are the occupying rates of octahedral and tetrahedral aluminum sublattices respectively.

It is easily found that the above formula becomes the Scherrer formula when $L_1 = L_2 = L_3 = L$, $a_A = a_B = 0$, $a_A = a_C = 0$ or $a_B = a_C = 0$.

The measured and calculated with the above formula integrated width have been listed in table 1, where $L_1 = 13.45$ nm, $L_2 = 2.37$ nm, $L_3 = 1.19$ nm. It can be seen that the calculated integrated width are in agreement with the measured ones for γ– alumina.

Table 1. Comparision of the measured and the calculated integrated width of γ– alumina.

HKL	MEAS.	CAL.
(111)	2.89	3.94
(220)	7.34	7.72
(311)	4.03	3.97
(222)	0.73	0.73
(400)	1.02	0.75
(511)	5.56	4.34
(440)	1.44	1.06
(444)	1.20	0.98

Besides, we proved that the structure defect has no influence on the x–ray diffraction integrated intensity. The calculated integrated intensities are in agreement with the measured ones either.

PS-12.01.33 THE TRANSLATION SYMMETRY IN QUASICRYSTALLOGRAPHY N. C. Shi*, Z. S. Ma, X- Ray Laboratory, China University of Geosciences, Beijing 100083, China

The quasicrystal is generally considered to lack translation symmetry, but it has long-range order in some crystallographic orientations. In order to describe a three dimensional framework or a two dimensional net in a quasicrystal, Penrose tiling was adopted. Penrose tilings were full of crystal space by matching and inflation (or deflation) operation, then they were decorated by Ammann lines. Penrose tilings are quite different from the symmetry operation of conventional crystallography which is composed of point symmetry, translation as well as combination of point symmetry and translation. Is it possible that quasilattices are deduced by the symmetry operation of coventional crystallography? In order to solve this problem, a new kind of scheme on the configuration of quasicrystal unit cell and deduction of quasilattices has been suggested by the symmetry operation of conventional crystallogaphy. For this kind of scheme, it is a key problem that the translation is defined as non-integral period translation, where the concept of incommensurable translation has been suggested. This method of the deduction of quasilattice is described in details as follows: 1. select the unit cell in a quasicrystal through Bravais principle; 2. analyse the fractal dimension character of quasicrystal and find the self-similarity proportion factor; 3. define the direction and length of the translation vector of the unit cell based on self-similarity proportion factor; 4. carry out incommensurable translation operation and point symmetry. The operations stated as above will lead to inflation or deflation of the pattern, and then the quasilattice is obtained. In the diffraction space, the result of deduction is consistent with the diffraction pattern in the icosahedral phase and octagonal phase.

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