

17-Symmetry and its Generalizations

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tallographic constraints (Pond R.C., *J. Crystal Growth*, 1986, 79, 946; Efimov A.N., Thesis, Leningrad, 1986) are presented for the case of negligible metric misfit.

As example an analysis of epitaxial defects was carried out for the structure "rhombic yttrium HTS 1-2-3 on SrTiO₃". Result is shown in table 1. All these types of defects was observed experimentally by using electron microscope technique.

Possibilities of single crystalline growth for rhombic yttrium HTS -crystal 1-2-3 on substrate with structure of distorted perovskite (Fesenko E.G., Perovskite family and ferroelectricity, Moscow, Atomizdat, 1972) are illustrated by table 2 (only planes (001), (010), (100) of reduced unit cell are considered).

Table 2.

Symmetry of reduced perovskite unit cell	(001)	(010)	(100)
Cubic	twinning	twinning	twinning
Tetragonal	twinning	single crystal	single crystal
Rhombic 1	single crystal	single crystal	single crystal
Rhombic 2	single crystal	twinning*	single crystal
Rhombohedral	twinning*	twinning*	twinning*
Monoclinic	single crystal	twinning	single crystal

* Polysynthetic twinning without incoherent interfaces is possible.

It is shown that defect-free heterocomposition should be created provided the translation groups of layer and substrate are in agreement meanwhile defects caused by the discrepancy between the point groups ought to be removed by the angular deflection of substrate plane from singular one.

PS-17.01.11 FREE SPACE CRYSTALLOGRAPHY AND THE VOLUME TERM OF GIBBS ENERGY: COMPARISON OF THREE PATTERNS OF HEPTAGONS!

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In many cases space filling is of interest in crystallography (Pauffler, Leuschner 1975). In this connection the study of gaps is relevant. Here the free space in three patterns of heptagons (generalization from 2-D nets to 3-D lattices is also performed) is investigated. Geometrical and physical peculiarities are considered. For instance the effect in volume term of the Gibbs energy (Leuschner 1979, 1989) is estimated.

PS-17.01.10 DETERMINATION OF LAUE SYMMETRY USING CONVERSE-TRANSFORMATION ANALYSIS. Vicky Lynn Karen* and Alan Mighell, Reactor Radiation Division, National Institute of Standards and Technology, Gaithersburg, MD 20899 USA.

Our newly-developed theory of Converse-Transformation analysis (*J. Appl. Cryst.* (1991) 24, 1076) permits symmetry, as a theoretical concept, to be abstracted directly from the experimental data. In practice, the Converse-Transformation matrices are calculated as soon as any unit cell has been determined. This new approach permits the collection of experimental data, the evaluation of experimental errors, the determination of metric symmetry and the assignment of the Laue symmetry with respect to ANY basis, no matter how skewed. The metric symmetry is deduced simply by counting; the greater the number of matrices, the higher the symmetry. All possible symmetries and pseudo-symmetries within any specified tolerance are immediately apparent. This is especially important in preliminary structure work and in protein crystallography where the experimental errors may be large. The Laue symmetry is assigned by using the Converse-Transformation matrices to generate sets of equivalent hkl's, then measuring and evaluating the intensities of the equivalent reflections. Mistakes in Laue symmetry are avoided since it is not necessary to do key experimental steps out of order. With this approach, all the data required to assign the Laue symmetry are collected before a conventional cell is determined. In contrast, procedures currently used in diffractometry are based on the risky practice of assuming a conventional cell and symmetry, and then collecting data to verify the assumption. This erroneous strategy may lead to the assignment of a Laue group of too low symmetry. This new method has many experimental applications including the automation of diffractometers and the editorial review of manuscripts prior to publication. Software for analyzing symmetry and for determining general lattice relationships may be obtained from Dr. Vicky Lynn Karen.