12-Amorphous, Imperfectly Ordered and Quasi-periodic Materials


It is well known that the static modulation of some incommensurate (IC) displacive phases evolves toward a soliton regime. The purpose of this work is to analyze from a theoretical point of view the influence of that evolution on the diffraction pattern. The temperature dependence of the atomic displacements are described in the frame of the Landau theory. A new expression for the structure factor of an IC displacive structure has been obtained. It explicitly includes the modulus and phase of the order parameter. From this expression it is predicted the sequential changes of both the main reflections and the satellites. In particular, it is shown that high order satellite reflections can be more intense than satellites of lower order. The specific order of these unexpectedly high-intensity satellites depends on the specific compound. Besides, it is shown how some previous experimental results, used as an evidence in favour of a phonon temperature factor, can be explained as a consequence of the changes in the static modulation. On the other hand, it has been obtained that, depending on the compound, there exist satellite reflections for which the ratio between their intensities only depends on the degree of anharmonicity of the modulation. Concerning the intensity of main reflections, it can be shown that some of them can strongly vary with temperature and even exhibit a pronounced minimum.

Finally, these predictions are compared with some experimental results found in two compounds that present a soliton regime: Thiourea (S(NH)2) and Rb2ZnCl4.


The modeling of 2D or 3D quasi lattice of octagonal system is summarized. 2D system is firstly proposed by Beeker [Chem. P. M. 1987, 23, 927-931], in which 2D homometricity is investigated in relation to the discovery of octagonal quasicrystals of NCOI (Bio, K.K. Phys. Rev. Lett. 1987, 59, 1010-1013) and related alloys. The modification of 2D tilings is shown by considering the rotation of 4D hyper-cubic lattice (Soma, T. & Watanabe, Y. Acta Crystal, 1992, A48, 470-474). In 3D case, quasicrystals with above six-fold rotational symmetry takes necessarily layer structure. However, it is necessary that pseudo-octagonal quasi-lattice without layer structure but with 6D network like a 3D Penrose tilings is possible to build. The case base vectors are chosen such that their projection has perfect eight-fold symmetry (Watanabe, Y. et al. Materials Science Forum 1987, 22-24, 214-222). It can be shown that a 3D quasi-periodic tiling could be generated by the projection of cubic lattice from the 72 space to 3D tiling space (Soma, T. et al. Quasicrystals and incommensurate Structure in Condensed Matter 1992, 10-21). The four kinds of unit cells, cube, square parallelogram, parallelogram, and rhombic parallelogram, are found.

by choosing independent triplets of base vectors. Self-similarity and its matching rule is also investigated for this 3D tiling (Watanabe, Y. et al. Proceedings of China-Japan Seminars 1989-1990, 204-211). The strategy of self-similar modeling is summarized. In this congress, self-similar transformation matrix of four kinds of unit cells and n-th generation matrix obtained by Computer Algebra are also presented, which is confirmed by the fact that ratios of the matrix element converge irrational number with a approach infinity.

PS-T.01.19 SUPERSPACE APPROACH TO INCOMMENSURATE INORGANIC MISFIT LAYER COMPOUNDS

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Inorganic misfit layer compounds are a class of incommensurate intergrowth compounds. They comprise two chemically different but close-packed layers, which are stacked alternately. The first type is a transition-metal dichalcogenide, i.e., T2O3, in which one of the layers, e.g., NiO or TiO2, is a close-packed layer, while the second layer, e.g., MoS2, is a pseudo-close-packed layer. The second type is a transition-metal monochalcogenide, MX, and can be considered as a two-layer thick (100) slice cut out of a rock-salt-type structure. Each of the two types of layers has an average periodic structure, which is incommensurate with the other lattice. It appears that for all misfit layer compounds b* and c* are the same for the two layer-types, while a* and a, have incommensurate length ratio. A corollary is the seemingly non-stoichiometric character of these compounds: (MX)2X3, with x ranging from about 1.1 to 1.2. The precise value of x depends on the ratio of the two unit-cell volumes.

The real structure of incommensurate intergrowth compounds consists of incommensurately modulated subsystems. Its analysis can be done most fruitfully using the superspace description and employing superspace groups to characterize its symmetry (Van Smaal, 1992). It will be demonstrated how the superspace description is used to classify the various stackings, as observed in the misfit layer compounds, and to analyze the specific features of the inter-subsystem bonding, as connected with the incommensurateness (Van Smaal and de Boer, 1992; Petricek et al., 1993).

References