12-Amorphous, Imperfectly Ordered and Quasi-periodic Materials

PS-12.01.17 INFLUENCE OF THE STRUCTURAL EVOLUTION OF AN INCOMMENSURATE DISPLACIVE PHASE ON ITS DIFFRACTION PATTERN.

I. Aramburu *, G. Madariaga and J.M. Pérez-Mato. Departamento de Física de la Materia Condensada. Facultad de Ciencias. Universidad del País Vasco. Apdo. 644, 48080 Bilbao, Spain.

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 sensitivity to structural 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 phason 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 ($SC(NH_2)_2$) and Rb_2ZnCl_4.

PS-12.01.18 QUASILATTICE OF OCTAGONAL SYSTEM OBTAINED BY PROJECTION AND SELF-SIMILAR METHOD

By Y.Watanabe* & T.Soma. The Institute of Physical and Chemical Research Wako-shi,Saitama 351-01, Japan.

The modeling of 2D or 3D quasilattice of octagonal system is summarized. 2D system is first proposed by Beenker (Beenker,F.P.M. TH Report 82-WSK-04, 1982, Eindhoven Technical Univ,The Netherlands) as a projection of 4D cubic lattice to 2D space. Afterwards, various 2D patterns are investigated in relation to the discovery of octagonal quasicrystals of NiCrSi (Kuo,K.H. 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 Cryst,1992,A48,470-475). In 3D case, quasilattice with above six-fold rotational symmetry takes necessarily layer structure. However, it is proved that a pseudo-octagonal quasilattice without layer structure but with 3D network like a 3D Penrose tiling is possible to build. In this case base vectors are chosen such that their projection has perfect eight-fold symmetry(Watanabe,Y.etal. 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 7D space to 3D tiling space (Soma,T.et al. Quasicrystals and Incommensurate Structure in Condensed Matter 1990,231-242). The four kinds of unit cells, cube, square-parallelogram-parallelepiped, rhombic-parallelogram-parallelepiped,rhombohedron,are obtained 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 elucidated. In this congress self-similar transformation matrix of four kinds of unit cells and n-th generation matrix obtained by Computer Algebra are given. Quasiperiodicity is confirmed by the fact that ratios of the matrix element converge irrational number with n approach infinity.

PS-12.01.19 SUPERSPACE APPROACH TO INCOMMENSURATE INORGANIC MISFIT LAYER COMPOUNDS

Jan L. de Boer* and Sander van Smaalen, Laboratory of Chemical Physics, University of Groningen, Nijenborgh 4, NL-9747 AG GRONINGEN, The Netherlands and V. Petricek, Institute of Physics, Academy of Sciences of Czech Republic, Cukrovarnicka 10, 162 00 Praha 6, Czech Republic.

Inorganic misfit layer compounds are a class of incommensurate intergrowth compounds. They comprise two chemically distinct types of layers, which are stacked alternatingly. The first type is a transition-metal dichalcogenide, TX_2, isostructural to a single layer in NbS_2 or TiS_2. The second type is a transition-metal monochalcogenide, MX, and can be considered as a two-atom thick (100) slice 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 $\mathbf{a}_1$ and $\mathbf{a}_2$ have incommensurate length ratio. A corollary is the seemingly non-stoichiometric character of these compounds: $(MX)_xTX_2$, 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 Smaalen, 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 analyse the specific features of the inter subsystem bonding, as connected with the incommensurateness (Van Smaalen and De Boer, 1992; Petricek et al., 1993).

References

S. van Smaalen (1992). Materials Science Forum, Vols. 100 & 101, 173-222.
S. van Smaalen and J.L. de Boer (1992). Phys. Rev. B46, 2750-2757.
V. Petricek, I. Cisarova, J.L. de Boer, W. Zhou, A. Meetsma, G.A. Wiegers and S. van Smaalen (1993). Acta Cryst. B49, in press.

