

**PS10.04.21 THE STRUCTURE MODULATION OF BI-BASED HIGH- $T_C$  SUPERCONDUCTORS.** A.A.Levin, Yu.F.Shepelev, Yu.I.Smolín, Institute of Silicate Chemistry, Russ. Ac. Sci., St.-Petersburg, Russia

The modulated structures of high- $T_C$  superconductors  $\text{Bi}_4\text{Sr}_4\text{CaCu}_3\text{O}_{14+x}$  (Bi-4413, orthorhombic cell,  $a = 5.411(2)$ ,  $b = 5.417(3)$ ,  $c = 27.75(1)$  Å,  $q = 0.213(4)b^*$ ,  $T_C^{\text{end}} = 84$  K) and  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$  (Bi-2212, orthorhombic cell,  $a = 5.407(3)$ ,  $b = 5.412(3)$ ,  $c = 30.771(8)$  Å,  $q = 0.210(2)b^*$ ,  $T_C^{\text{end}} = 75$  K) are determined in both commensurate and incommensurate approximations utilizing single-crystal X-Ray diffraction data.

The modulation displacement functions of all atoms in the structures are obtained. It has been found that the oxygen atoms of BiO layers in both compounds have greatest modulation shifts along the b-axis (up to 1.20 Å in Bi-2212 and up to 1.40 Å in Bi-4413) and their modulation functions in this direction can be described by linear saw-like functions. It is shown that the extra-oxygen atoms can be inserted in the BiO layers of the structures.

The modulation of the structures, the topology of the BiO layers and the form of the modulation displacement functions are explained by the models of shifts of the oxygen atoms in the BiO layers correlated according to antiferroelectrical law. The difference of modulation models of the Bi-2212 and Bi-4413 structures are discussed. The marked peculiarity of both structures is a rather great concentration of the vacancies in Sr positions adjacent of copper-oxygen layers. It is suggested that the cationic vacancies in the Sr sites provide the hole conductivity in the copper-oxygen layers and lead to the formation of a percolation network in the superconducting crystals.

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**PS10.04.22 MOSSBAUER DIFFRACTION IN CRYSTALS WITH INCOMMENSURATE MODULATION.** E.N.Ovchinnikova, Moscow State University, Physical Department, Moscow 119899, Russia

A set of possible reflections was considered for a case of Mossbauer resonant diffraction in incommensurately modulated crystals with quadrupole interaction on nuclei. A structure, formed by electrical field gradients (EFG) on Mossbauer nuclei supposed to be modulated too. We believe, that atomic displacements in a modulation wave are enough small and they cause mainly the rotation of EFG main axes. Our propositions are based on the results of the published earlier NMR studies of EFG's in incommensurate ionic crystals. In this case a quasicontinuous distribution of quadrupole splittings exists, and EFG tensors on nuclei can be considered as a sum of EFG's corresponding to an average structure and additional modulation tensors. These approximations were used to study the features of Mossbauer diffraction pattern. A simple harmonic law of modulation was used. It was shown, that the diffraction pattern consists of main Bragg reflections and satellites. It differs from x-ray diffraction pattern in those cases, when purely nuclear Bragg reflections occur. Satellites of purely nuclear reflections are also purely nuclear. Their energy spectra are broaden doublets. Energy forms of all other reflections and their satellites are determined by interference between potential and resonant scattering. The satellite reflections energy spectra contains an information about additional modulation tensors. We have considered incommensurate phases of some crystals containing Mossbauer isotopes, in which the discussed phenomena may be observed.

**PS10.04.23 DYNAMICAL SCALING AND DIFFUSE SCATTERING DURING POLYTYPIC TRANSITIONS.** Dhananjai Pandey and S. P. Shrestha, School of Materials Science and Technology, Banaras Hindu University, Varanasi-221005, India.

We discuss here the application of zero temperature non-conserved dynamics on 1d Ising chains for calculating the evolution of diffuse scattering during martensitic transitions between polytype structures like 2H, 3C, 4H and 6H using Monte-Carlo technique. For the simulations, we have mapped these structures into model magnetic systems. We have used 1d Ising Hamiltonians with pairwise interactions extending upto third neighbours. The introduction of deformation faults during transitions has been mapped into spin flip dynamics. It is shown that the pair correlation functions exhibit dynamic scaling at late stages. The diffuse scattering patterns obtained by taking the Fourier transforms of pair correlation functions are shown to be in good qualitative agreement with those observed on ZnS single crystals. It is shown that the evolution of diffuse scattering patterns at late stages of these transitions is completely determined by a single characteristic length scale ( $\xi$ ). It is found that irrespective of the initial and product phases involved,  $\xi$  shows a power law dependence on time with a universal exponent of 0.5. It is proposed that polytypic materials may serve as model systems for experimentally verifying the dynamical scaling behaviour of equal time pair correlation functions predicted theoretically for 1d stochastic systems.

**PS10.04.24 MISFIT LAYER COMPOUNDS  $(\text{SbS})_{1.15}(\text{TiS}_2)_n$  WITH  $n=1,2$ .** Y. Rena<sup>a</sup>, A. Meetsma<sup>a</sup>, S. van Smaalen<sup>b</sup>, V. Petricek<sup>c</sup>, C.H. Ruecher<sup>d</sup>, C. Haasa<sup>a</sup>, and G.A. Wiegers<sup>a</sup>. <sup>a</sup>Chemical Physics, University of Groningen, 9747 AG Groningen, The Netherlands; <sup>b</sup>Lab for Crystallography, University of Bayreuth, 95440 Bayreuth, Germany; <sup>c</sup>Institute of Physics, Czech Academy of Sciences, 16200 Praha 6, Czech Republic; <sup>d</sup>Institute for Mineralogy, University of Hannover, 30167 Hannover, Germany.

The incommensurate crystal structures of the misfit layer compounds have been determined on the basis of a (3+2)-D superspace-group using single crystal X-ray diffraction. The structures are built up by alternating stackings of double layers SbS and single or paired sandwiches  $\text{TiS}_2$ . The SbS double layers consist of an intrinsic interface modulation. The distinguishing feature is the incommensurate ordering of Sb/S atoms on the distorted rock-salt structure of SbS, which results in Sb-Sb and S-S clusters. The electronic structure has been studied using photoelectron spectroscopies. 22% of the total Sb atoms are in Sb-Sb contacts. All spectrum peaks are broadened by the mutual interaction of the two subsystems. The top valence band consists mainly of S 3p states and the conduction band of Ti 3d states. The study of their electrical transport and optical properties shows a 2D Fermi-liquid behaviour.