12-Amorphous, Imperfectly Ordered and Quasi-periodic Materials

PS-12.01.14 CRYSTAL STRUCTURE OF SECOND INCOMMENSURATE PHASE OF BETAINE CALSIUM CHLORIDE DIHYDRATE. By M.Machida*,Y.Miura and N.Achiwa, Department of Physics, Kyushu University, Higashi-ku, Fukuoka, Japan.

Betaine calsium chloride dihydrate(BCCD) exhibits a complicated phase sequence with two incommensurate phases modulated along the c axis;the incommensurate phases are stable in the temperature regions 164K-127K(INC1, $\gamma > 2/7$) and 125K-116K(INC2, $2/7 > \gamma > 1/4$) (Brill,W. and Ehses,K.H.,Jpn.J.Appl.Phys.,1985,**24**,826.). We have investigated the crystal structure of the INC2 phase of BCCD at 122K using the (3+1)-dimensional formalism for the modulated structure. The superspace group was assumed to be $P(\ Pnma\ )$:($1,s,-1$) ($\gamma = 0.278$) on the basis of the extinction conditions and result of the pyroelectric measurement made by Ribeiro and Almeida (Ribeiro,J.L. and Almeida,A.,Phys.Rev.,1989,**B39**,320.). The intensity data, including main and first-order satellite reflections, were measured by the ω scan technique. Independent reflections with $F_o \geq 3\sigma(F_o)$ were used in the structure refinement. Only the first-order harmonics was taken into consideration in the modulation functions. Final reliability factors were R=0.058 for the whole 2494 reflections and R_s = 0.098 for the first-order 1386 satellite reflections. The result of present structure analysis indicates that ordinary single-mode modulation is acceptable for the structure of the INC2 phase in the first-order harmonics approximation.

PS-12.01.15 TEM STUDIES ON MODULATED STRUCTURES IN 2223 PHASE WITH $Bi_{1.6}Pb_{0.4}Sr_2Ca_2Cu_3O_y$ COMPOSITION. By S.S.R. Inbanathan, G. Singh, Department of Physics, Banaras Hindu University, Varanasi - 221 005, India.
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Recently, it has been shown (D.Pandey,A.K.Singh and A.P.Singh, Physica C, 1992, 204,179) that single phase 2223 can be prepared within a total heat treatment duration of 48 hrs by a novel semi-wet route using $Pb_{0.2}SrCa(CO_3)_{2.2}$ precursor. We present here the nature of modulated structures observed in such single phase samples using TEM techniques. In the Pb substituted 2223 phase, modulation wavelengths ranging from about 6.5b to 9b have been reported in the literature (O.Eibl, Physica C, 1991,175,419) for different Pb contents. This is in marked contrast to the modulation wavelength of nearly 4.7b in Pb free samples.

In our single phase samples, all the grains analyzed by selected area electron diffraction patterns revealed a modulation wavelength of nearly 7.2b as shown in Fig.1. This indirectly confirms that the semi-wet samples possess homogeneous distribution of Pb. In fact, x-ray line broadening analysis of the pure diffraction profiles has also revealed that the distribution of various cations in different grains is quite homogeneous since a plot of $\beta\cos\theta$ versus $\sin\theta$ is found to have zero gradient within experimental errors (β is the FWHM and θ the Bragg angle). This is further confirmed by HREM studies which show uniform fringe spacing of nearly 7.2b as shown in Fig.2. The undulations in this figure are due to the atomic columns aligned and tilted with respect to the incident beam. Twist boundaries with a and b axes interchanged are ubiquitous in these samples.

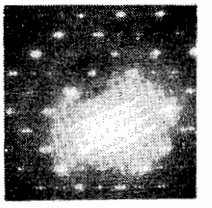

Fig.1. [001] SAD pattern showing modulation along b^*

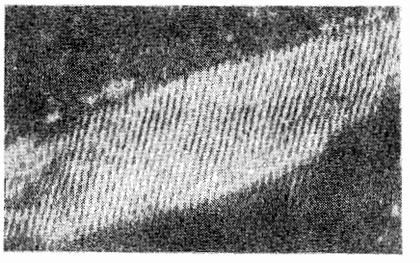

Fig.2. Darkfield lattice image with incident beam|| [001]

PS-12.01.16 THE LANTHANIDE OXIDE FLUORIDE AND ZIRCONIUM NITRIDE FLUORIDE SOLID SOLUTIONS DESCRIBED AS COMPOSITE MODULATED STRUCTURES. By R.L.Withers*. S.Schmid and J.G.Thompson, Research School of Chemistry, Australian National University, GPO Box 4, Canberra City, ACT 0200, Australia.

It is shown that the only generally applicable crystallographic approach to the anion excess, fluorite-related solid solution fields reported in the zirconium nitride fluoride, uranium nitride fluoride and lanthanide oxide fluoride systems is a composite modulated structure approach. A TEM and powder XRD study has been made of the ZrN_xF_{4-3x} ($0.906 < x < 0.936$) system and the appropriate superspace group symmetries characterizing the Q and H sub-structures shown to be P : Abmm :1s-1($q_Q = -c_Q^* + [c_H^* - c_Q^*]$) for the Q sub-structure and B : Pmcm : s1-1 ($q_H = {}^1/_2 b_H^* + [c_H^* - c_Q^*]$) for the H sub-structure respectively. Fourier decomposition of the previously reported conventional superstructure refinement of one member of this solid solution field, $Zr_{108}N_{98}F_{138}$, has provided both underlying parent sub-structures as well as an approximation to the Atomic Modulation Functions (AMF's) describing the mutual influence of the two parent sub-structures upon each other. In addition, such a Fourier decomposition has given an indication of the sorts of problems that will inevitably be encountered in accurately determining the appropriate AMF's when a conventional superstructure refinement of such composite modulated structures is attempted.

