s1.m1.p5 **Analysis of the Weissenberg diffraction images from Bi2212, using Fuji imaging plate and Synchrotron X-ray.** T.J. Lee[1], T.S. Khor[1],, William Chen[1], Li Yang[2], Z. H. Wan[2] and H.F. Fang[2]. *1.Department of Physics, National Tsing Hua University, Hsin-Chu 300, Taiwan, R.O.C. 2.Institute of Physics, Chinese Academy of Science, Beijing 100080, P. R. China*
Keyword: incommensurate, structure, Bi2212.

Diffraction patterns of "TSFZ grown Bi2212 crystals" were obtained using lΔ synchrotron X-ray from KEK, Japan. Diffraction intensities are collected, using Weissenberg camera equipped with Fuji imaging plates. The crystal structure exhibited one dimensionally incommensurate modulation along b direction with modulation wave vector $\mathbf{q} = 0.243\mathbf{b}^* + \mathbf{c}^*$. Determination of the structure parameters of this "one-dimensionally incommensurate modulated structure" was carried out by automatic search on 4-dimensonal Fourier maps. Structure model will be built according to the resultant Fourier maps. The structure and functional relation will be interpreted with the resultant model.

s1.m1.p6 **Ab initio study of incommensurately modulated crystals.** R.Caracas and X.Gonze, *Université Catholique de Louvain, B-1348, Louvain-la-Neuve, Belgium.*
Keywords: aperiodic, incommensurate, band structure.

We present the ab initio study of the average structures of some incommensurately modulated materials: K_2SeO_4 , $Sn_2P_2Se_6$, Mo_2S_3 , $AuTe_2$ (calaverite) and Pb_2MgTeO_6 (elpasolite).All the calculations are done using the local density approximation (LDA) and/or the general gradient approximation (GGA) of the density functional theory. We focused up to now on the caracterization of the static properties of these average structures. The electronic band structure, the corresponding Density-Of-States and the valence electron density distributions are determined for all the materials. Three-dimensional representations of the valence electron density distribution helped to identify the important structural groups present in the structures and the chemical bonds between the atoms. Partial valence electron density maps are generated in order to link the electronic bands to different atomic orbitals or to linear combinations of atomic orbitals. The K_2SeO_4, $Sn_2P_2Se_6$, and Pb_2MgTeO_6 are good isolants with large electronic gaps. For all these three materials, the electron band structure is made of weakly-dispersive electronic bands. The Mo_2S_3 and $AuTe_2$ present a metallic character. Consequently for these two materials the Fermi surface has been also analysed in order to find the instabilities and possible nesting vectors of the Fermi surface.

Results of the ab initio determination of the average structure are also reported. The quality of these results, compared to the experimental data, are very material-dependent, the final results varying within 1 and 10 % difference to the experiment. For $AuTe_2$ the LDA gave differences to the experimental data of the order of 6-8%, while the GGA improved considerably the quality of the results, reducing the differences up to 3-4%. For Mo_2S_3 LDA is within 2% while for the other materials the agreement lies between the one for $AuTe_2$ and the one for Mo_2S_3.

The next main step of the project will be the determination of the phonons in order to find out the instabilities of the average structures.