increases with higher concentration of antimony. The analysis of diffraction patterns of BaPb<sub>0.7-x</sub>Sb<sub>x</sub>Bi<sub>0.3</sub>O<sub>3</sub> points to increase in the tilt angle of (Pb,Bi,Sb)O<sub>6</sub> octahedrons with increased concentration of antimony. The a and c crystal lattice parameters and the volume of BaPb<sub>0.7-x</sub>Sb<sub>x</sub>Bi<sub>0.3</sub>O<sub>3-δ</sub> unit cell linearly decrease with the increase in the x index up to x = 0.3. The measured a and c parameters do not depend on the x for x > 0.3. Electrical resistivity rapidly increases for x > 0.3. The binding energy of Pb4f and Bi4f levels in XPS spectra can be measured only for x < 0.3, because the photoelectric lines are broader and splitted above this value. Therefore we conclude that the upper limit of Pb replacement by Sb is equal to 0.3. Scanning electron microscopic observation and energy dispersive X-ray analysis (EDS) show second phase that crystallizes among BaPb<sub>0.7-x</sub>Sb<sub>x</sub>Bi<sub>0.3</sub>O<sub>3-δ</sub> grains. This phase isolates the grains and causes that resistivity rapidly increase for the samples with x > 0.3. The BaPb<sub>0.7</sub>-<sub>x</sub>In<sub>x</sub>Bi<sub>0.3</sub>O<sub>3-δ</sub> compounds crystallize in I4/mcm tetragonal structure. Measured a and c crystal lattice parameters as well as the volume of the unit cell decrease with the increase of indium content but non-linear decrease of the aand c parameters is observed. The measured lattice parameters are constant for x > 0.2. Electrical resistivity rapidly increases for the x parameter higher than 0.2 as well as the width of the Bi4f, Pb4f and Sb3d photoelectric lines. It points that the upper limit for Pb replacement by In in  $BaPb_{0.7-x}In_xBi_{0.3}O_{3-\delta}$  is for x = 0.2. Applying different techniques we discuss relations among crystal structure, electronic structure and physical properties in the BaPb<sub>0.7-x</sub> $M_x$ Bi<sub>0.3</sub>O<sub>3- $\delta$ </sub> (M = Sb, In) system.

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#### MS25 P13

The relation between symmetry and the FTIR spectra of the kaolinite and dickite, M. Zamama<sup>a</sup> and M. Berraho <sup>a</sup>, Department of Chemistry, University of Marrakech, Morocco. E-mail: <u>zamama@ucam.ac.ma</u>

## Keywords: Kaolin, symmetry, FTIR

The structural analysis of the clay minerals is more difficult than that of the almost perfect crystals. In the case of the phyllosilicates, the particle sizes which constitute the material are so smalls to be studied by the monocrystals method which gives precise structural information. In the other hand, the hydrogen atoms position is uncertain and conflicting results was published about the symmetry mode when we take into account the hydrogen atoms coordinates (1,2). The present study concerns the kaolinite and dickite which are polytypes and belong to the phyllosilicates family. The corresponding structural formulas of one half of the unit cell are, respectively, Al<sub>2</sub> Si<sub>2</sub>O<sub>5</sub>(OH)<sub>4</sub> and Al<sub>4</sub> Si<sub>4</sub>O<sub>10</sub>(OH)<sub>8</sub>. This material, is described as a stacking of the layers witch consists of a tetrahedral and the octahedral sheets sharing a common plan of oxygen atoms and hydroxyl groups. The polar nature of the structure, with hydroxyls on the one surface of the layer and the oxygen atoms at the other surface, allows hydrogen bonds to form between the adjacent layers. The OH groups play an important role in the attraction between the layers. Little information are known about the strengths and the nature of the hydrogen bonds in those particular structures. The infrared spectroscopy gives indications on the orientation of the OH groups and the corresponding absorption bands in the infrared spectrum depends strongly on the defects existing in the mineral. For this raison, the position of hydrogen atoms in the structure is important. In this study, our aims is to distinguish between the structure of dickite and kaolinite. In order to predict the infrared spectrum for the OH groups, we propose to specify the environment of the hydroxyls groups according to the symmetry. The experiments of the intercalation (3) demonstrate that OH groups frequencies are sensitive to the variation of the  $d_{001}$ distance. For this reason, we consider that the environment of the hydroxyl groups is determined essentially by the symmetry of the interfoliar space. We have constructed two fundamental entities: the tetrahedral sheet and the octahedral sheet. This analysis is made in 3 stages with decreasing symmetries: we consider the models of the perfect crystal, the crystal with a deformed layers and the symmetry of the real crystal. We have determined that the P3 symmetry of the interfoliar space symmetry is conserved in the perfect crystal and the crystal with a deformed layers. On basis of this symmetry, the FTIR spectra are discussed and compared to the spectrum of the real crystal.

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#### MS25 P14

Anomalous X-ray Scattering and absorption spectroscopy Investigate the Morphology of FePt Monolayer Nanoparticle on Surface Modified Substrates, Tzu-Wen Huang, Kuan-Li Yu, Yen-Fa Liao and Chih-Hao Lee aDepartment of Engineering and System Science, National Tsing-Hua University, Hsinchu, Taiwan, National Synchrotron Radiation Research Center, Hsinchu, Taiwan.

 $E\text{-mail: }\underline{chlee@mx.nthu.edu.tw}$ 

### Keywords: FePt nanoparticle, X-ray absorption spectroscopy, Anomalous Grazing Incident Small Angle X-ray Scattering

The structural stability of self-assembled FePt monolayer nanoparticles on functional substrate with the Au overlayer during the annealing were studied. To deposit a monolayer of particles under control, the functional substrates such as polyethylenimine (PEI) or [3-(2aminoethlyamino)ropyl] trimethoxysilane (APTS) modified silicon wafers were used to capture the FePt nanoparticles coated with oleic acids. With the X-ray diffraction, anomalous X-ray absorption spectroscopy and the anomalous grazing incidence small angle x-ray scattering techniques, the FePt nanoparticles monolayer were found to be free from coalescence and convert into ordered alloy under the annealing process after 5-10 nm of Au overlayer deposited on the top of FePt nanoparticles. The result indicates that the particle size 4.5±0.5 nm is typically unchanged, but the distance between particles is reduced from 7.5±1.5 nm to 5.5±1.1 nm after annealing. The results suggest that the 5 nm Au coverlayer is an effective diffusing barrier layer to prevent the FePt

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nanoparticles from sintering during the annealing process. The ordered FePt(001) diffraction peak was obscured

under the strong Au background, but its X-ray absorption spectrum shows an order FePt structure was formed.

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