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**Keywords:** lattice anomalies, square lattice, frustration

#### P.11.01.10

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#### Comparison and Analysis of the Samples with Same Synthesis of Bi-Sr-Ca-Cu-O, Prepared by Different Ways of Heating

Basilis Papadopoulos<sup>1</sup>, C. Stergiou<sup>2</sup>, A. Stergiou<sup>1</sup>, <sup>1</sup>Department of Physics, <sup>2</sup>Department of Electrical & Computer Engineering, Aristotle University of Thessaloniki (A.U.Th.). Thessaloniki, Greece. E-mail: stergiou@auth.gr

For the study of superconducting materials, produced by different ways of heating, five mixtures with proportions 2:2:2:3 of Bi<sub>2</sub>O<sub>3</sub>, SrCO<sub>3</sub>, CaCO<sub>3</sub>, CuO were prepared. The four of them were heated, directly, at 860°, 870°, 880° and 890° C, individually, while the last one, gradually, at the same temperatures. All the samples were heated in free atmosphere, for 48h.

The crystalline phases, created in the eight cases, were studied by XRD measurements and characterized, using the PDF2 database. Further, the Powder Profile Analysis (Rietveld's method) was used for the crystallographic study of the samples. The phase Bi<sub>2</sub>CaSr<sub>2</sub>Cu<sub>2</sub>O<sub>8</sub>, with space group A<sub>maa</sub> and mean unit cell parameters a=5.4028, b=5.3923 c=30.6559 [1], was the main phase for all the samples, with a percentage greater than 80%. Some other phases with percentage 5-15% for the different samples were defined, say the Bi<sub>2</sub>SrCuO<sub>5</sub>, with structure analogous of Dy<sub>2</sub>BaCuO<sub>5</sub> [2] (Pnma space group and mean unit cell parameters a=12.2020, b=5.6732, c=7.1357).

Results of the samples synthesis for each of the processes were discussed.

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**Keywords:** superconductors, crystal structure, Rietveld's method

#### P.11.01.11

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#### Crystallographic Study of Superconducting series Nd<sub>1+x</sub>Ba<sub>2-x</sub>Cu<sub>3</sub>O<sub>y</sub> (x=0.0, 0.2, 0.4, 0.6), Prepared at 850°C and 860°C

C. Stergiou<sup>1</sup>, G. Voutsas<sup>2</sup>, A. Stergiou<sup>2</sup>, <sup>1</sup>Department of Electrical & Computer Engineering, <sup>2</sup>Department of Physics, Aristotle University of Thessaloniki, Thessaloniki, Greece. E-mail: stergiou@auth.gr

The structural properties of superconducting series Nd<sub>1+x</sub>Ba<sub>2-x</sub>Cu<sub>3</sub>O<sub>y</sub> (x=0.0, 0.2, 0.4, 0.6), prepared at 850°C and 860°C, were studied. For this aim, four powder mixtures with suitable proportions of Nd<sub>2</sub>O<sub>3</sub>, BaO and CuO were prepared and heated at temperature 850° and next the produced samples were reheated at 860°C, in free atmosphere for 48h, in both cases. The creation and the evolution of the phases, as a function of the quantity x, was studied by analysis of XRD measurements. The phase characterization was realized with a suitable program, using the PDF2 data-base. Farther, the Powder Profile Analysis (Rietveld's method) was used for the phase structure refinement and the exact determination of the phase percentages. Four crystal phases, NdBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> [1], Nd<sub>2</sub>BaCuO<sub>5</sub> [2], BaCuO<sub>2</sub> [3] and CuO [4], were defined for the samples prepared at 850°C, while only the first three of these were defined for the samples prepared at 860°C. The creation and percentages of the crystal phases in the samples were discussed, as a function of the temperature and the quantity x.

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**Keywords:** superconductors, crystal structure, Rietveld's method

#### P.11.01.12

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#### Crystallographic Study of Samples Produced from Mixtures La<sub>1+x</sub>Ba<sub>2-x</sub>Cu<sub>3</sub>O<sub>y</sub> (x=0.0, 0.2, 0.4, 0.6), Heated at 850°C and 860°C

Semir Yilmaz<sup>1</sup>, C. Stergiou<sup>2</sup>, A. Stergiou<sup>1</sup>, <sup>1</sup>Department of Physics, <sup>2</sup>Department of Electrical & Computer Engineering, Aristotle University of Thessaloniki. Thessaloniki, Greece. E-mail: stergiou@auth.gr

Four powder mixtures with suitable proportions of La<sub>2</sub>O<sub>3</sub>, BaO and CuO according to general type La<sub>1+x</sub>Ba<sub>2-x</sub>Cu<sub>3</sub>O<sub>y</sub> (x=0.0, 0.2, 0.4, 0.6), were prepared and heated at temperature 850° and next the produced samples were reheated at 860°C, in free atmosphere for 48h, in both cases.

The creation and the evolution of the phases, as a function of the quantity x, was studied by analysis of XRD measurements. The phase characterization was realized with a suitable program, using the PDF2 data-base. Farther, the Powder Profile Analysis (Rietveld's method) was used for the phase structure refinement and the exact determination of the phase percentages.

Three crystal phases (the superconducting La<sub>1.76</sub>Ba<sub>0.24</sub>CuO<sub>4</sub> [1] and LaBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> [2], and the non superconducting BaCuO<sub>2</sub> [3]), were defined for all the samples. The creation and percentages of the crystal phases in the samples were discussed, as a function of the temperature and the quantity x.

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**Keywords:** superconductors, crystal structure, Rietveld's method

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#### Growth and Structural Investigations on lead-doped NdMnO<sub>3</sub> Single Crystals

H.L. Bhat<sup>a</sup>, Nilotpal Ghosh<sup>a</sup>, Suja Elizabeth<sup>a</sup>, G. Nalin<sup>b</sup>, B. Muktha<sup>b</sup>, T.N. Guru Row<sup>b</sup>, <sup>a</sup>Department of Physics, Indian Institute of Science, Bangalore-560012, India. <sup>b</sup>Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore-560012, India. E-mail: hlbhat@physics.iisc.ernet.in

Single crystals of Nd<sub>(1-x)</sub>Pb<sub>(x)</sub>MnO<sub>3</sub> with different dopant concentrations were grown by high temperature solution growth technique using PbO-PbF<sub>2</sub> flux [1]. Electron diffraction patterns showed the presence of superlattice structure x=0.25 and above. The structure of Nd<sub>(1-x)</sub>Pb<sub>(x)</sub>MnO<sub>3</sub> crystals were determined by single crystal x-ray diffraction for two different x values using a Bruker AXS Smart Apex CCD diffractometer with MoK $\alpha$  radiation. Positional co-ordinates of Nd and Mn atoms were obtained by SHELXS97 and refined by SHELXL97. Substitution of Pb at Nd site results in structural change from tetragonal (x=0.25) to cubic (x=0.38) lattice. The lattice parameters of tetragonal and cubic unit cells are a = b = 7.725(1)Å, c = 3.884(1) Å and a = b = c = 7.737(2) Å respectively. While the unit cell volume of tetragonal structure (P4/mmm) is comparable to that of parent NdMnO<sub>3</sub>, the volume of cubic unit cell (Pm3m) is doubled. The static distortion of MnO<sub>6</sub> octahedra is maximum for parent orthorhombic NdMnO<sub>3</sub> (x = 0). The mismatch between different Mn - O bond lengths of Nd<sub>1-x</sub>Pb<sub>x</sub>MnO<sub>3</sub> is much less at x = 0.25 and 0.38. The MnO<sub>6</sub> octahedral distortion and inter octahedral tilt are removed progressively with higher doping. Changes in transport properties as a function of temperature at different doping levels are in accordance with the structural changes.

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#### P.11.03.2

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#### Atomic Image of Diluted Magnetic Semiconductor Zn<sub>1-x</sub>Mn<sub>x</sub>Te Obtained by X-ray Fluorescence Holography

Shinya Hosokawa<sup>a</sup>, Naohisa Happo<sup>b</sup>, Kouichi Hayashi<sup>c</sup>, Toru Ozaki<sup>a</sup>,