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for living cells proliferations, and could reveals the piezoelectric properties, which arise in its noncentrosymmetric monoclinic phase $P2_1$. The hexagonal crystal structure of HAP with $P6_3/m$ symmetry is centrosymmetric and not manifested piezoelectricity. Here we report the computational studies of the structural, dielectric, elastic and piezoelectric properties for both HAP crystal structures symmetries. The first principles calculations, modeling and computer simulations were made using as semi-empirical PM3 method as well ab initio and DFT calculations (from HyperChem 8.0 and AIMPRO codes). These computational studies show that HAP crystal cell parameters are different for two symmetries and phases along the main c-axis, that provide the varieties of HAP nano-films widths in this direction (which could be revealed experimentally, e.g. by atomic force microscopy). The calculated values of elastic constants are close to known experimental data for both HAP group symmetries and confirm the existence of piezoelectricity for $P2_1$. The calculated small total energy difference for $P6_3/m$ and $P2_1$ leads to opportunity of coexistence for both phases.

P.89	**Electric and piezoelectric properties of the lead-free solid solution Ba0.85Ca0.15Ti1-xZrxO3 (0.1≤ x ≤0.2)** Maria-Elena Villafuerte-Castrejón[1], Salvador Rea-López [1], Armando Reyes Montero [1], Rigoberto López Juárez [2], Amador González Crespo [3], Álvaro García Lucas [4], Lorena Pardo Mata [4] [1]Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, México, D.F., Mexico, 04510; [2]Centro de Ciencias Aplicadas y Desarrollo Tecnológico, Universidad Nacional Autónoma de México, México, D.F., Mexico, 04510; [3]EUIT Telecomunicación, Technical University of Madrid, Spain; [4]Instituto de Ciencia de Materiales de Madrid, ICMM-CSIC, Madrid, Spain

Lead zirconate-titanate ceramics (PZT) are the most widely used piezoelectric materials to date, because of their high piezoelectric response, large scale production capability and the tailoring of their properties through composition. Nevertheless, the PZT is now restricted by the toxicity of the Pb, and therefore, there is an urgent need to develop lead-free piezoceramics. Very recently, a high-performance Pb-free piezoelectric system Ba0.85Ca0.15Ti1-xZrxO3 (BCTZ), has been reported, showing a very high d33 of 50-600 pC/N. It is also important the synthesis method selected, because of its influence on the grain size and then on the sintering conditions in order to obtain high density, homogeneous ceramics.In the present work the synthesis of Ba0.85Ca0.15Ti1-xZrxO3 (0.1≤ x ≤0.2) ceramics was performed by Pechini method; the crystalline powders were obtained after calcinations at 600° C, 700° C, 750° C, and 800° C. The powders were sintered at several temperatures and their electric properties have been measured by impedance spectroscopy. The piezoelectric properties have been evaluated using an iterative method of analysis of the resonance. Improved values of piezoelectric parameters as well as permittivity and dielectric losses are presented.

P.90	**Advance engineered piezoelectric materials for energy harvesting devices** Xin Wan[1,2], Ruud Steenwelle[1], Minh Duc Nguyen[1], Evert Houwman[1], Matthijn Dekkers[1], Dave H.A. Blank[1], Guus Rijnders[1] [1]MESA+ Institute for Nanotechnology, University of Twente, Enschede, Netherlands, 7500 AE; [2]IMEC/Holst Centre, IMEC/Holst Centre, Eindhoven, Netherlands

Piezoelectric materials offer a number of advantages in energy harvesting systems, by transforming ambient vibration into electrical energy, which can be stored and power other devices. To improve energy harvesting device performance, the figure of merit (e_{31}^2/ε) is vital to achieve a higher piezoelectric voltage and maximum the power output.

In this study, $Pb(Zr_{1-x}Ti_x)O_3$ (PZT) was chosen for its prime piezoelectric properties, such as their high piezoelectric coefficients, high power output density and relatively low epsilon. Epitaxial PZT thin films with controlled orientations are achieved on silicon substrates by pulsed laser deposition (PLD). $Pb(Zr_{1-x}Ti_x)O_3$ thin films with variety of dielectric constant (ε) and piezoelectric coefficient (e_{31}, d_{33}), were studied and compared with each other. We found very large figure of merit values within these engineered piezoelectric thin films. Using optimized composition, crystal orientation and strain, maximum values of 20.4 ±3 C/m^2 were found.. A shift of morphotropic phase boundary (MPB) is observed in the perovskite thin film structure, which is due to the residual strain caused by the different thermal expansion coefficients between PZT thin films and silicon substrates. These results show that for epitaxial PZT thin films, the composition of the PZT should be optimized to compensate the strain state. Besides the characterization of material properties, energy harvesting devices are also being fabricated and will be discussed in the contribution.

P.91	**Electro-optical piezoelectric fibres based on PLZT compositions: Synthesis and characterisation** Frank J. Clemens[1], Lujan Kozielski[2], Jiri Erhart[3] [1]Laboratory for High Performance Ceramics, 3EMPA, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland, 8600; [2]Department of Materials Science, University of Silesia, Sosnowiec, Poland, 41-200; [3]Technical University of Liberec, Czech Republic, 461 17

Lantanium doped PZT is well known as an electro-optical material. In the 70th such material was developed for anti-flash goggles. For future application this materials, in form of fibres will be very interesting for transducer application. Enhanced functionality of electro-optic devices are proposed by implementing piezoelectric micro fibers into composite construction. In this study different doped PLZT fiber with a diameter of around 300 micron were produced by thermoplastic processing method and disks were pressed by conventional uniaxial dry pressing method. The materials where sintered in PbO and PbZrO3/ZrO2 atmospheres to avoid lead loss in the material at different temperatures and dwell times. Finally the microstructural properties of fiber and pressed bulk materials were investigated by SEM analysis. Additionally from all materials phase analysis by XRD was investigated. As expected, the microstructure (grain size and porosity) and phase composition are influenced by the sintering conditions. To investigate the electro-optical properties fibre with the lowest porosity 0.5% and a grain size of 3.7 micrometer was used. The phase purity was investigated by the XRD pattern and Rietveld analysis. The light-induced impedance and piezoelectric coefficient was investigated at relatively low light intensity (below 50 mW/cm^2). By applying a UV LED, a piezoelectric change constant of 219 C/N could be observed.

P.92	**Grain size effects on dielectric and piezoelectric properties of piezoceramics under compressive stress** Diego A. Ochoa, Jose E. García Department of Applied Physics, Universitat Politècnica de Catalunya, Barcelona, Spain, 08034

In many applications, piezoceramics operate under compression stress. When these materials are subjected to usual prestress of designed devices, functional properties display significant changes. Moreover it is well known that grain size reduction notably affect piezoceramic properties by dropping their functionality. Exploring grain size effects on properties of piezoceramics under prestress should contribute to improve design of