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Structural and electrical properties of $Ba_{0.85}Ca_{0.15}Ti_{0.9}Zr_{0.1}O_3$ ceramics

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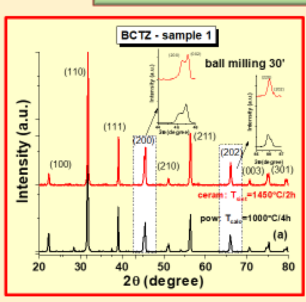
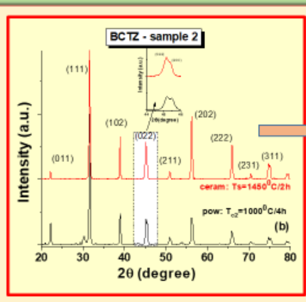
Aim of the present work

- To prepare $Ba_{0.85}Ca_{0.15}Ti_{0.9}Zr_{0.1}O_3$ ceramics by solid state reaction using conventional ceramic processing, applying different grinding ways: 1) ball-milling (BCTZ 1) and 2) manual (BCTZ 2). The ceramic samples were subject to a different calcination step and after that they were sintered at the same temperature of 1450°C for 2h.
- A comparative study of electrical properties for low and high electric fields (dielectric permittivity at different temperature and frequency range, $P(E)$ hysteresis loops and dc-tunability).
- To investigate the effect of electric poling on the structural and piezoelectric properties of the BCTZ samples .

Structural characterization by: - XRD

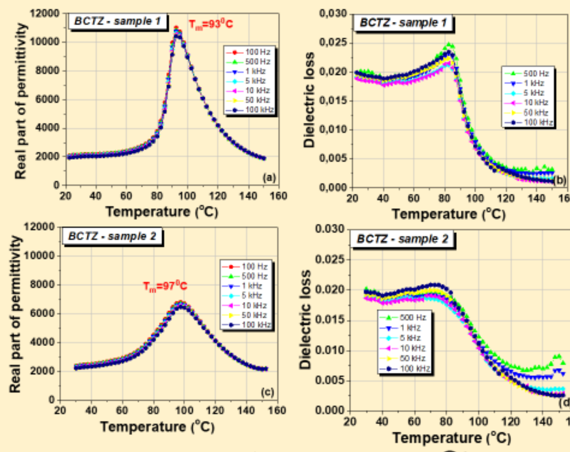




- X-ray analysis indicated a superposition of phases with a highlighted phase belonging to the tetragonal structure, for BCTZ 1.

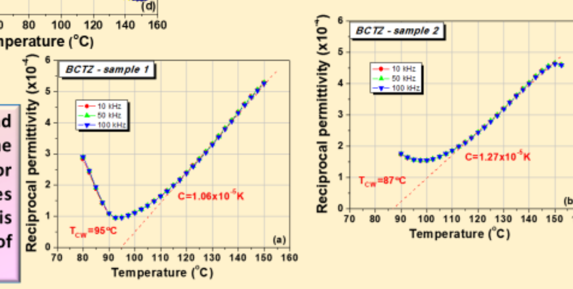
- the 2nd BCTZ ceramic sample presents orthorhombic structure even for calcinated powder and sintered ceramic.

Dielectric properties - Phase transition behavior



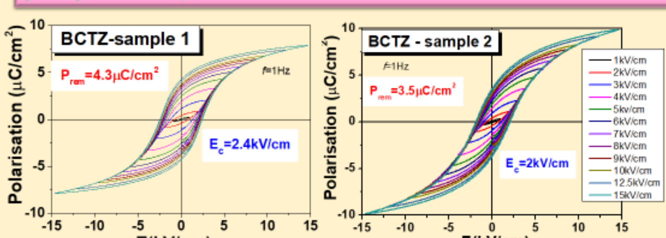
- At room temperature, both BCTZ samples present almost similar permittivity (ε) value of ~2000, with dielectric losses of about 2%, which are indicating a good dielectric character.
- The presence of ferro-para phase transition, with a sharp increase of permittivity to 11000 at T_m=93°C for BCTZ1, and a more diffuse one with smaller permittivity maximum value of 6800 at a slightly higher temperature of T_m=97°C for frequency of 100Hz.

- The Curie-Weiss analysis for the dielectric permittivity data:



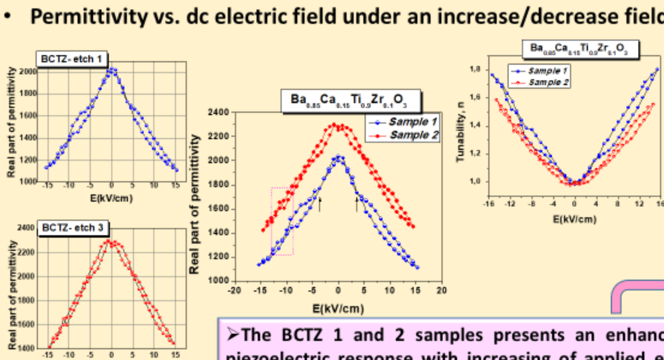
- The difference between the Curie-Weiss and the temperature corresponding to the maximum permittivity (difference of 2°C for sample 1 and 10°C for the sample 2) indicates that at local level the BCTZ sample 2 is characterised by a higher degree of inhomogeneity than BCTZ 1.

High field properties (ferroelectric, tunability and piezoelectric properties)

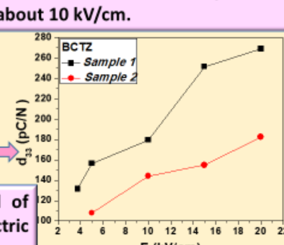


- The switching characteristics present a reduction of the coercitivity field from 2.4 to 2kV/cm, remnant polarization (P_r) from 4.3 to 3.5 μC/cm² and area, in BCTZ sample 1 and BCTZ sample 2, respectively.

- Permittivity vs. dc electric field under an increase/decrease field cycle



- The dc electric field dependence of tunability indicates an interesting feature (change of trend) for a dc field of about 3.75 kV/cm and about 10 kV/cm.

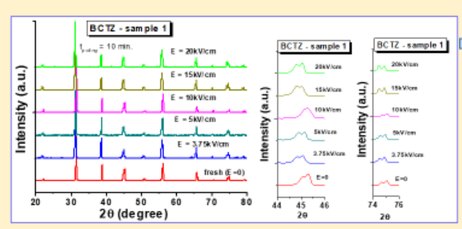


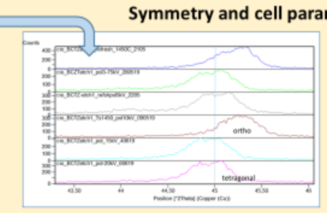
- The BCTZ 1 and 2 samples presents an enhanced of piezoelectric response with increasing of applied electric field.

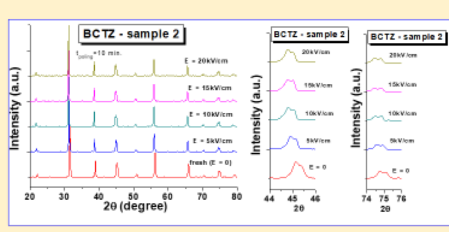
Structural modifications induced by poling

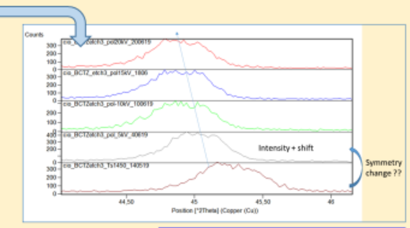
- Structural calculations and simulations

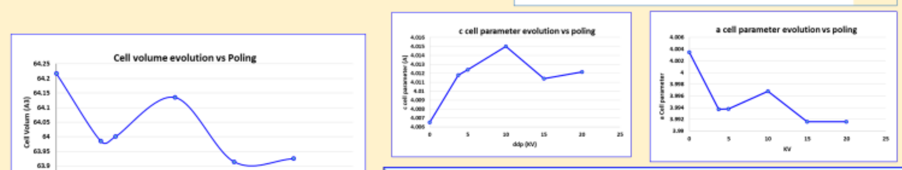
Symmetry and cell parameter evolutions











- Structural cell parameter changes were noted for 5 and 10kV/cm applied electric field.

Conclusions

- The phase composition and the functional properties of $Ba_{0.85}Ca_{0.15}Ti_{0.9}Zr_{0.1}O_3$ ceramic samples are strongly affected by the mixing strategy of the precursor powders in the synthesis phase, which is reflected on the degree of compositional and structural homogeneity of the ceramics.
- The XRD analysis and Rietveld calculations have indicated Tetragonal and Orthorombic structure for BCTZ sample 1, BCZT sample 2 respectively.
- By applying different electric fields on the BCTZ samples, it was observed that the crystalline symmetry can be modify.
- The permittivity vs. temperature indicates the presence of ferro-para phase transition, with a sharp increase of permittivity to 11000 for BCTZ sample 1, and a more diffuse one for BCTZ sample 2.
- The diminishing of dielectric permittivity in BCTZ sample 2 is a result of combined intrinsic phenomena with the structural perovskite distortion, which can cause also the reduction of the polarisation (poor ferroelectricity) in these two types of BCZT samples.

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