

International workshop *Physics and mechanics of random structures: from morphology to material properties*

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3D modelling of ferroelectric composite properties using X-ray micro tomography images: Effective permittivity and tunability

D. Bernard^{1,2}, C. Elissalde^{1,2}, C. Estournès³, J. Lesueur^{1,2}, E. Plougenven^{1,2}, and M. Maglione^{1,2}

¹*CNRS, ICMCB, UMR 5026, F-33600 Pessac, France*

²*Univ. Bordeaux, ICMCB, UMR 5026, F-33600 Pessac, France*

³*CIRIMAT et Plateforme Nationale CNRS de Frittage Flash, PNF2 MHT, Univ. Paul Sabatier, F-31062 Toulouse, France.*

Ferroelectric materials are widely used for microelectronic applications and different approaches are explored to produce new materials with well-controlled properties (permittivity, Curie temperature, dielectric losses, tunability, ...). In the composite approach we selected, dielectric particles are introduced in a ferroelectric powder to obtain, by Spark Plasma Sintering (SPS), a composite with dielectric inclusions distributed within a ferroelectric matrix. Optimisation of the process relies on diverse characterization methods and different numerical methods.

This presentation focussed on the final step where, for the same samples, permittivity and tunability have been measured and computed using X-ray Computed Micro Tomography (XCMT) images as input. We first exposed the microscopic problem verified by the potential at the microstructure scale, the scale at which the real material has been characterised by XCMT. Then, it is shown that the model we developed reproduces the permittivity anisotropy induced by the deformation of the dielectric inclusions due to SPS.

For tunability (permittivity variation with the applied electric field) we begin by introducing Johnson's law as constitutive law, then we derived the dimensionless form of the problem putting into evidence its main parameters. Fitting numerical results with experimental ones, it is shown that this simple law allows reproducing the experimental data with a very good precision, but, surprisingly with the introduction of an anisotropic coefficient of nonlinearity. Consequences of this second kind of anisotropy are discussed.

Finally, the effects on the dielectric properties of various changes in the morphology of the samples are explored in order to extract the dominant ones.