

## BASIC INFORMATION ON SUB-PROJECT

NAME OF PROGRAMME/FUND	Scholarship Fund - Sciex NMS <sup>ch</sup>
RESEARCH FIELD AND OTHER RESEARCH FIELDS INVOLVED (if applicable)	Physics
TITLE OF THE SUB-PROJECT	(NANODO2) Domain walls in complex BaTiO <sub>3</sub> /SrTiO <sub>3</sub> nanostructures.
REGION OF THE CZECH REPUBLIC (according to the location of the home institution)	Prague
GRANT AMOUNT SPENT	34 561,45 CHF
INTERMEDIATE BODY	Swissuniversities
HOME INSTITUTION	Institute of Physics, Academy of Sciences of the Czech Republic
HOST INSTITUTION	EPFL, Materials
NAME OF THE FELLOW	Vilgelmina Stepkova
ABSTRACT OF THE SUB-PROJECT	<p>The idea of this project is to use phase-field simulations aimed to guide the design of artificially grown heterostructures capable to stabilize desired types of dense domain structures at nanometric scales. It is believed that particular geometrical arrangement of ferroelectric BaTiO<sub>3</sub> and dielectric SrTiO<sub>3</sub> should induce domain arrangements, which have interesting functional properties. We wish to use the experience from the related NANODO1 project (proposed in parallel to this present project, by my colleague Petr Ondrejko<sup>v</sup>ic), which is focused on clarification of defect-domain wall interactions in nanotwinned BaTiO<sub>3</sub> and to extend the modelling to the medium with sharp BaTiO<sub>3</sub>/SrTiO<sub>3</sub> interfaces. We hope to design geometries accessible to thin-film and related laboratory technologies so that the results can be actually probed experimentally in nearest future.</p>

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### MAIN RESULTS

BaTiO<sub>3</sub> nanorods embedded into SrTiO<sub>3</sub> were studied using phase-field simulation method. As expected, the ferroelectric properties of BaTiO<sub>3</sub> nanorods are markedly different from the BaTiO<sub>3</sub> bulk. It was shown that BaTiO<sub>3</sub> cylindrical nanorods embedded into paraelectric SrTiO<sub>3</sub> matrix maintain ferroelectricity up to 380 K. The ground state of the rods is rhombohedral due to mechanical clamping by SrTiO<sub>3</sub>. The stable structure of 10-80 nm diameter nanorods have closed-circuit quadruplet domain configurations. Interestingly, the out-of-plane polarization can be switched without perturbing the vortex arrangement of in-plane polarization components. Moreover, the in-plane clockwise or anticlockwise component of the polarization can be reversed by inhomogeneous electric fields, therefore the chirality of closed-circuit quadruplets could be exploited as an independent information stored in each nanorod. In principle, such heterostructures could be grown by thin-film technologies. The results of this research work have been published in Physical Review B: Rapid Communications [1].

[1] V. Stepkova, P. Marton, N. Setter, and J. Hlinka, Closed-circuit domain quadruplets in BaTiO<sub>3</sub> nanorods embedded in a SrTiO<sub>3</sub> film, Phys. Rev. B 89, 060101(R) (2014).

DATE OF REALISATION OF THE FELLOWSHIP

15.4.2013 - 14.10.2013

MORE INFORMATION ON THE PROGRAMME

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