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Sonderforschungsbereich 595

Elektrische Ermüdung in Funktionswerkstoffen

TECHNISCHE UNIVERSITÄT DARMSTADT

Sonderkolloquium
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Controlling the electrical properties of polar ABO_3 perovskites: are we in control?

This talk will focus on the influence of chemical doping and non-stoichiometry in three perovskites; ferroelectric $BaTiO_3$ (applications in multi-layer capacitors); charge ordered $Ba_2Bi^{3+}Bi^{5+}O_6$ (superconductor when doped with K on the A-site or Pb on the B-site); and piezoelectric $Na_{1/2}Bi_{½}TiO_3$.

In the case of $BaTiO_3$, the experimental results of Rare Earth (RE^{3+}) doped materials are verified by atomistic simulations using a recently updated potential set based on a model that includes covalency that exists between the Ti and O atoms [1]. The simulations offer an exciting tool for analysing local strain effects and provide the opportunity to observe the small, sometimes subtle, local alterations that occur in the $BaTiO_3$ lattice [2, 3]. They also confirm the so-called RE donor-doping mechanism does not exist for samples prepared in air; instead the electronic conductivity arises from oxygen-loss associated with high temperature processing.

In the case of $Ba_2Bi_2O_6$ we demonstrate how to suppress the electronic conductivity associated with mixed Bi^{3+} and Bi^{5+} ions on the B-site to generate non-ferroelectric, high permittivity oxides utilising lone pair Bi^{3+} and d^o Nb^{5+} ions on the B-site [4].

Finally, we discuss the remarkable influence of the Na:Bi A-site starting ratio on the conduction properties of $Na_{½}Bi_{½}TiO_3$. In this case we use a combination of Impedance Spectroscopy, electro-motive force (emf) measurements and O^{18} Tracer Diffusion measurements to prove the existence of (unexpected) high levels of oxide ion conduction in Bi-deficient compositions.

Finally, we discuss the question posed in the title and highlight the important roles that modelling, chemical doping and material processing conditions play in targeting the desired electrical properties.

Der Vortrag findet um **16:00 Uhr** im Gebäude der Materialwissenschaften, Lichtwiese, Petersenstr. 23, **Raum 228** statt