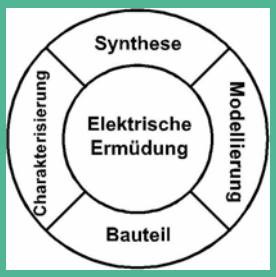

Sonderforschungsbereich 595

Elektrischer Ermüdung in Funktionswerkstoffen

TECHNISCHE UNIVERSITÄT DARMSTADT

Kolloquien im WINTERSEMESTER 2007/2008

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Modeling surfaces, interfaces and compositional order in ferroelectric materials

The cubic perovskite oxides ABO3 show great promise for the development of new materials having improved ferroelectric and electromechanical properties by tuning their chemical composition. The solid solutions with stoichiometric substitutions of the A or B metal atoms, like PZT, PZN or PMN-PT, are some of the promising examples. Based on ab-initio density functional calculations we propose that it may also be possible to optimize desired materials properties by additionally tuning the degree and type of compositional order in these compounds. Artificially layered structures with different cations which compositionally break the inversion symmetry of the perovskite structure might be especially exciting and fruitful in this regard. The resulting asymmetry of the ferroelectric double-well potential in such a material suggests the prospect of qualitatively new behavior, e.g., ``self-poling" materials.

In the second part of the talk I will address how surfaces and interfaces, e.g., domain walls, influence the ferroelectric properties of prototype cubic perovskite compounds. In particular the question, whether an intrinsic critical thickness exists, below which ultrathin films loose their ferroelectric properties, will be discussed, an issue which is very important for the application of ferroelectric thin films in semiconductor devices.

Die Vorträge finden, wenn nicht anders angegeben, jeweils um **16:15**
im Gebäude der Materialwissenschaften, Lichtwiese, Petersenstr. 23, **Raum 77** statt