ICAMS INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION	**RUB-SEMINAR** ***MATERIALS SCIENCE AND TECHNOLOGY***	Institut für Werkstoffe Institute for Materials

Period: Summer Term 2024

Time: Thursday, June 20, at 12.00
Venue: RUB, ZGH seminar room 03-121

Dr. Frank Wendler

Friedrich-Alexander-Universität, Fürth

will give the seminar

A novel approach to parametrize a ferroelectric phase-field model from atomistic simulation data

Abstract: Phase-field simulations based on the Landau-Ginzburg-Devonshire theory extend the time and length scales in comparison to molecular dynamics (MD) simulations. The interpretation and adaption of the continuum model parameters is not trivial, but crucial for a correct upscaling of MD results from ideal and defective ferroelectric single crystals.

MD simulations using a core-shell potential for polarization switching in ferroelectric barium titanate (BTO) with and without vacancy defects are carried out. Crucial material properties such as elastic and piezoelectric tensor components, kinetic coefficients, as well as domain wall characteristics are extracted from the MD data to adjust the anisotropic gradient energy. To generate a complete energy landscape, a proposed parametrization workflow involves determining all coefficients for the 6th order Landau polynomial from polarization reversal characteristics. Polarization switching in BTO involves localized nucleation and subsequent domain growth, driven by an applied electric field. MD simulation data proves the role of thermal activation in domain nucleation, resulting in a notable scatter in coercive fields within small systems. From statistic analysis of this data we calculate the activation parameters for BTO that govern polarization switching at coercive fields not only for perfect, but also those containing vacancy defects, and the domain wall energies. An approach comparable to the nudged elastic band method is applied in the phase-field simulations to probe the barriers by transitions over the critical nucleus.

The method is important for phase-field simulations of domain nucleation and domain wall motion in presence of point defects carrying mono- or dipolar electric fields as well as elastic strain fields, and for the motion and interactions of multiple domain walls.

Host: Prof A. Grünebohm, ICAMS, RUB

The *Materials Science and Technology Seminar* is jointly organized by the *IM* (Institute for Materials) and *ICAMS* (Interdisciplinary Centre for Advanced Materials Simulation). Members of the *RUB Materials Research Department MRD* and of the *DGM Regionalforum Rhein-Ruhr* are cordially invited to participate in the seminar. For further information please contact: Dr. Manuel Piacenza, icams@rub.de, phone: +49 234 32 25480.

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