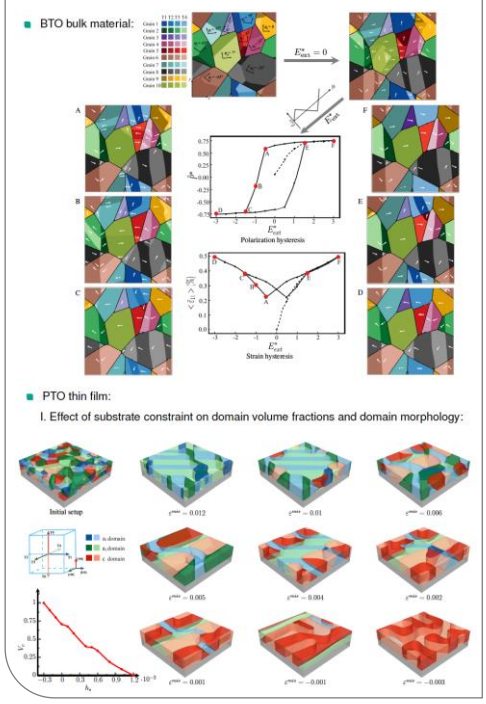
Master Thesis

Phase-field simulation studies of domain morphology evolution in perovskite ferroelectric semiconductor

Background and Tasks:

Pervskite ferroelectric semiconductor demonstrates remarkable electronic properties, particularly evident at domain walls, positioning it as a highly promising material for advanced photovoltaic applications. It has been observed that the stability of vertical domain structures significantly impacting its properties. Using an newly developed multiphase-field approach to study domain structures in ferroelectric materials [1], the goals of this work are to theoretically compute and analyze the stability of the in-plane domains, develop strategies for controlling the vertical domains, investigate the influence of the mechanical driving force as well as the electric driving force on the domain morphology, and explore the impact of grain morphology on domain structures and associated photoelectric phenomena in a perovskite ferroelectric semiconductor.

Previous simulation results



Requirements:

Basic knowledge in material science and physics is advantageous for handling the topic. Interest in numerical simulations, and in familiarizing oneself with new methods and subject areas, should be present.

We offer:

- Intensive supervision
- Modern workstations and high-performance computers as working environment
- Productive and dynamic atmosphere within a team
- Collaborations with international research groups
- Career prospects as junior researchers

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Reference:

[1] L. Fan, M. Reder, D. Schneider, M. Hinterstein, and B. Nestler. A phase-field model for ferroelectric materials—based on the multiphase-field method. Comput. Mater.Sci., 230:112510, 2023.