Atomistic scale finite element method for the simulation of ferroelectric functional materials

Introduction

Ferroelectric functional materials are simulated on all length scales. Especially atomistic simulations have been developed further over the last decades. Therefore atomistic simulations are not only used to predict material behaviour but also help understanding material behaviour in general. Ferroelectric phenomena, like e.g. domain walls can be simulated accurately by atomistic simulations. In order to reduce the computational costs of atomistic simulations we propose a molecular static finite element algorithm.

Molecular statics - finite elements

Considering a discrete particle system of N particles the total energy of the system is given by the sum of internal and external potential energies

$$E^{tot} = \Phi^{int}(\mathbf{r}) + \Phi^{ext}(\mathbf{r}) = \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N}\Phi^{int}(\mathbf{r}_{ij}) + \sum_{i=1}^{N}\mathbf{f}_i \cdot \mathbf{r}_i.$$

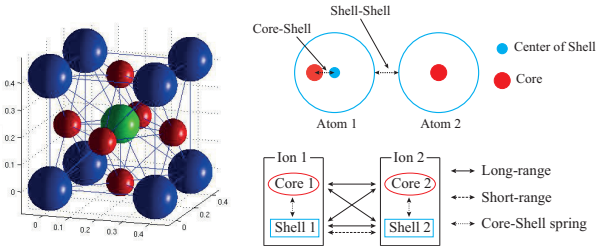
Minimization of the total potential energy leads to an equilibrium configuration

$$\frac{\partial E^{tot}}{\partial \mathbf{r}} = \mathbf{0}.$$

Interpreting and discretizing every interaction as a one-dimensional nonlinear truss element a discrete particle system can be solved in the same spirit as a nonlinear FE problem.

Core-Shell model

In the core-shell model every ion in the crystal lattice is modeled by two particles: the first particle represents the positive charged atom core whereas the second particle represents the negative charged electron shell of the ion [1].



Three different interaction potentials are considered [2]:

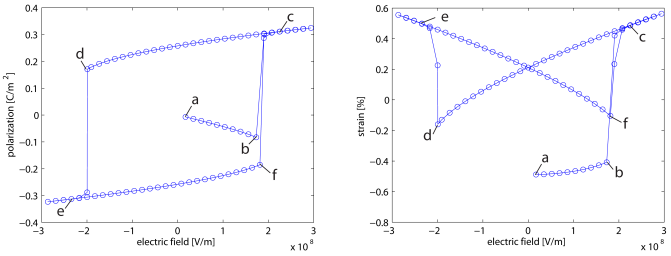
$$V_{\mathbf{r}_{ij}}^{Coulomb} = \frac{q_i q_j}{4\pi\epsilon_0 |\mathbf{r}_{ij}|}$$

$$V_{\mathbf{r}_{ij}}^{Buck} = A\exp\left(\frac{|\mathbf{r}_{ij}|}{\rho}\right) - \frac{c}{|\mathbf{r}_{ij}^6|}$$

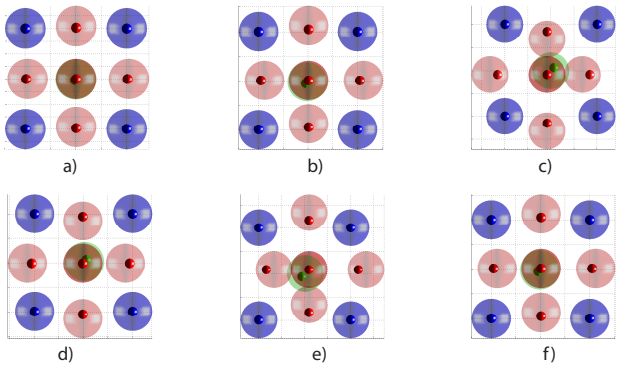
$$V_{\mathbf{r}_{ij}}^{Spring} = \frac{1}{2}k_2|\mathbf{r}_{ij}^2| + \frac{1}{24}k_4|\mathbf{r}_{ij}^4|$$

Ferroelectric hysteresis behaviour

As numerical example we calculated the ferroelectric hysteresis behaviour of ferroelectric barium titanate.



Starting from a ideal cubic and unpolarized reference configuration, the hysteresis firstly follows a metastable equilibrium path until it switches to the stabil path at b. These results agree with theoretical considerations [3].



Additional to the calculation of the ionic polarization of the unit cells we are also able to observe the electron polarizations of the ions.

Future challenges

Including temperature for non 0K conditions as well as detailed simulations of microscopic material behaviour at domain walls and system boundaries are future challenges of molecular statics. Furthermore multiscale coupling with methods like e.g. quasi-continuum method or FE^2 are promising applications for molecular static finite elements methods.

References

[1] S. Tinte et al., *J. Phys.: Cond. Mat.* 11: 9679 - 9690, 1999.
[2] M. Sepliarsky et al., *Curr. Opin. Solid State Mater. Sci.* 9:107 - 113, 2005.
[3] R. Landauer, *J. Appl. Phys.* 28:277, 1987.

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