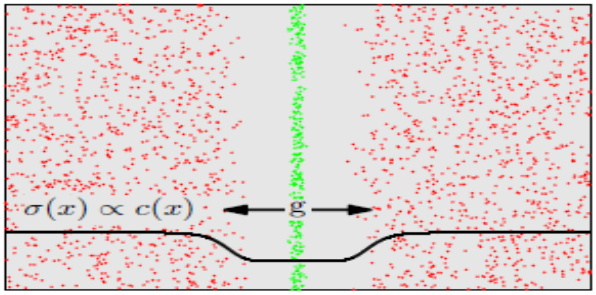
Master thesis project in Computational Physics

Monte Carlo and space charge formation

The aim with the project is to solve a combined statistical mechanics and electrostatic problem in three dimensions using the Monte Carlo method.

The overall conductivity in proton conducting oxides is most often limited by high-resistance grain-boundaries. The physical mechanism that causes the high resistance is believed to be due to space charge effects. At present the standard model for the space charge formation in oxides is based on a mixed continuum and discrete treatment, it assumes a one-dimensional geometry and it uses a mean field approach for the electrostatic interactions. The aim with this master thesis project is to improve on this.



In the project you will combine theory and computations, and get training in modeling and analyzing complex processes in materials.

More precisely you should:

1. Introduce a three-dimensional discrete model describing a grain-boundary system.
2. Implement the screened Coulomb interaction for a periodic system in an efficient way.
3. Take segregation energies and dielectric screening properties from DFT results.
4. Solve the model for the charge distribution and the electrostatic potential using the Monte Carlo method.
5. Study the effect of the segregation energy for the electrostatic potential and concentration profile both perpendicular and parallel to a grain-boundary plan.
6. Compare with the traditional Poisson-Boltzmann description and try to improve on that type of description.

The project is suitable as a 30 hp master project, for one or two students. Useful background are computational physics and statistical mechanics. You should have an interest in modeling and a good background in combining theory and computations.

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