Aalto University

Multiscale method for simulating KPFM

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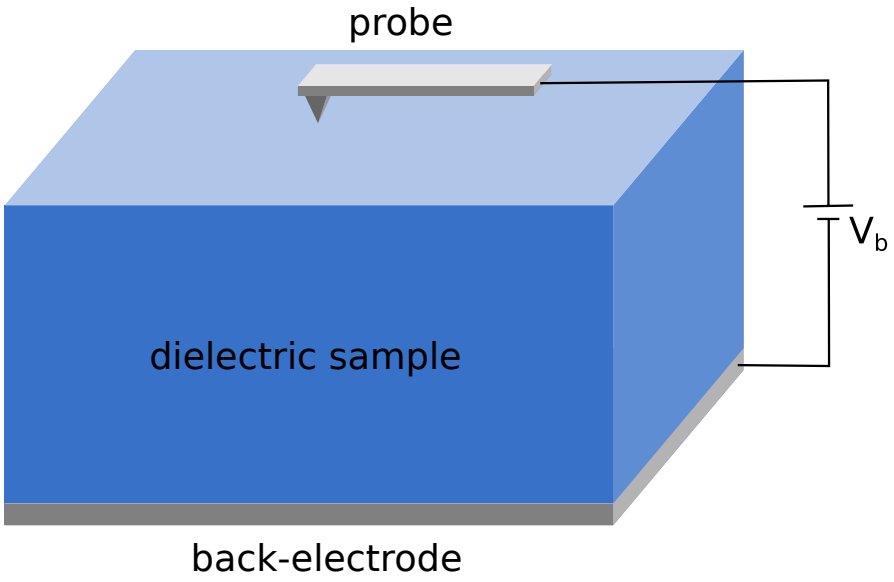
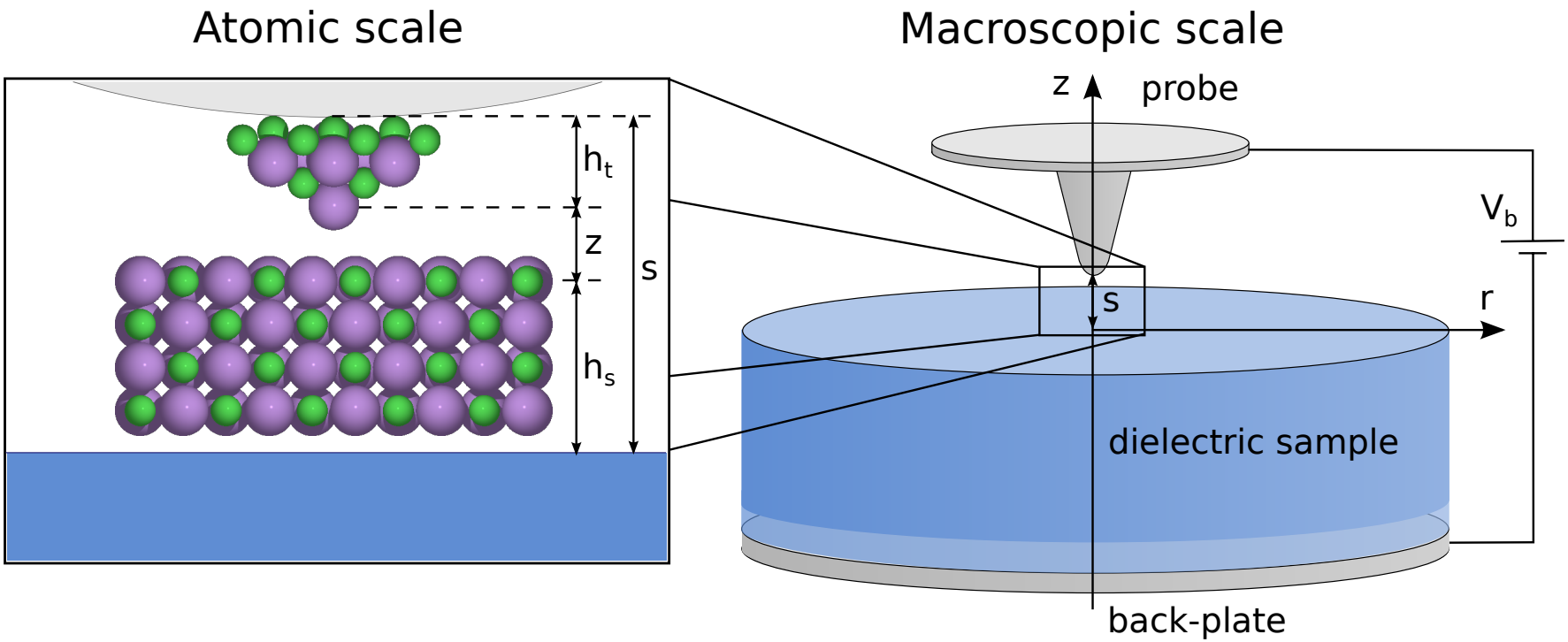
KPFM measurement setup

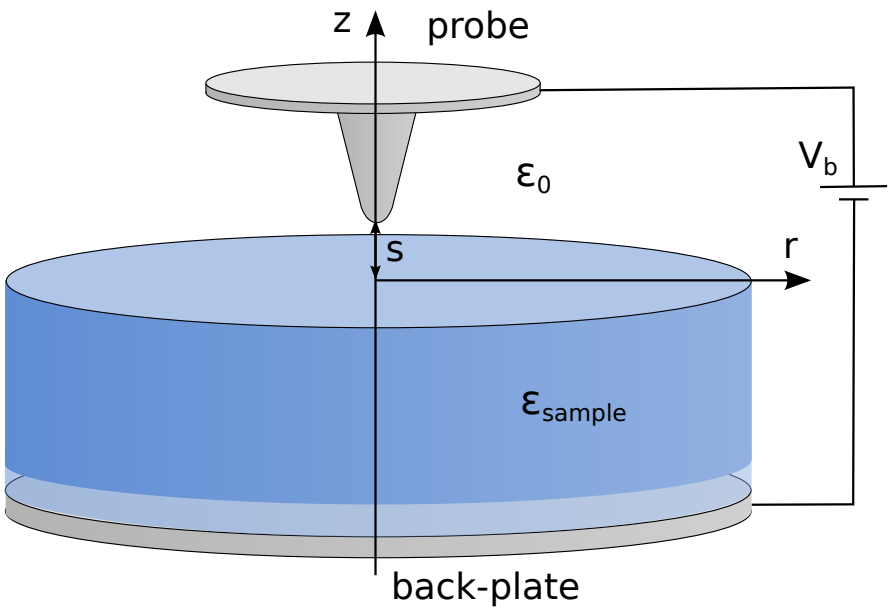


- The interesting quantity: $F_{probe}(x, y, z, V)$
- Effective bias voltage: $V = V_b - V_{CPD}$
- Sample is thick, considered as bulk material

Two length scales

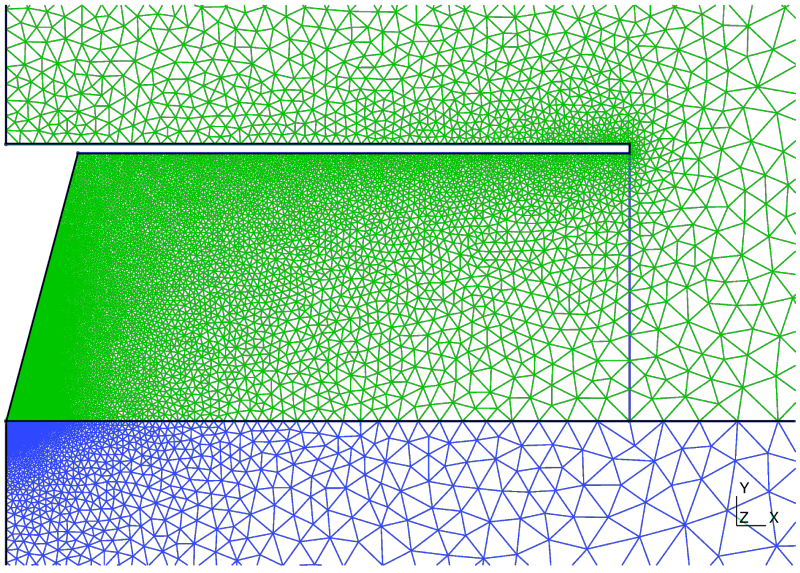


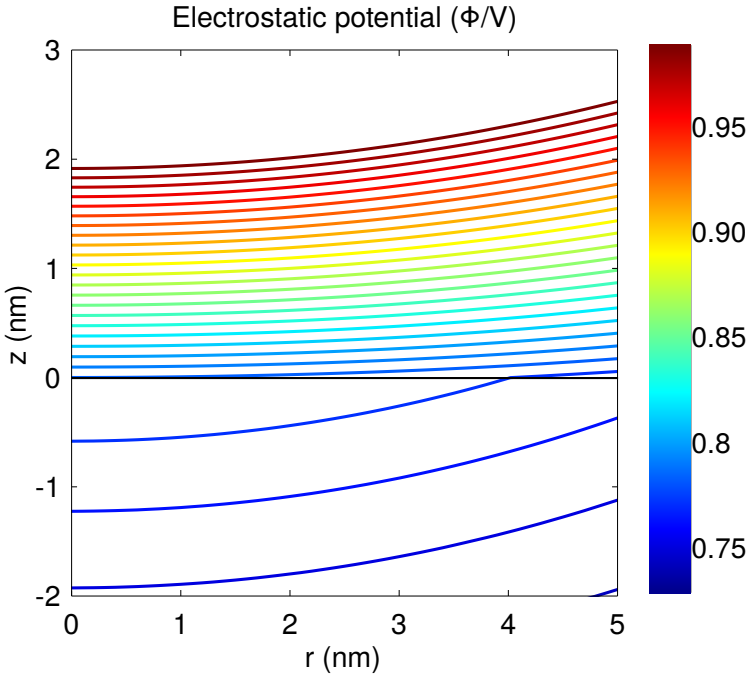
Macroscopic model



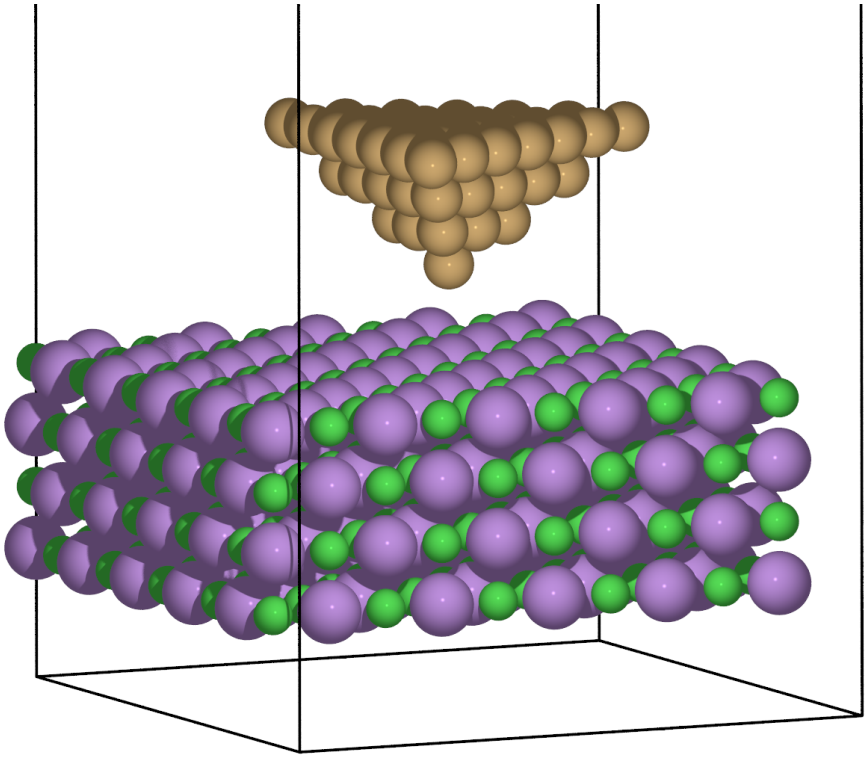
- Axisymmetric model of the probe
- Classical electrostatic boundary value problem
- Solve electrostatic potential $\Phi(\mathbf{r})$ from generalized Poisson equation $\nabla \cdot [\epsilon(\mathbf{r}) \nabla \Phi(\mathbf{r})] = 0$
- Boundary values: $\Phi_{probe} = V$, $\Phi_{backplate} = 0$

Solving electrostatic potential using FEM



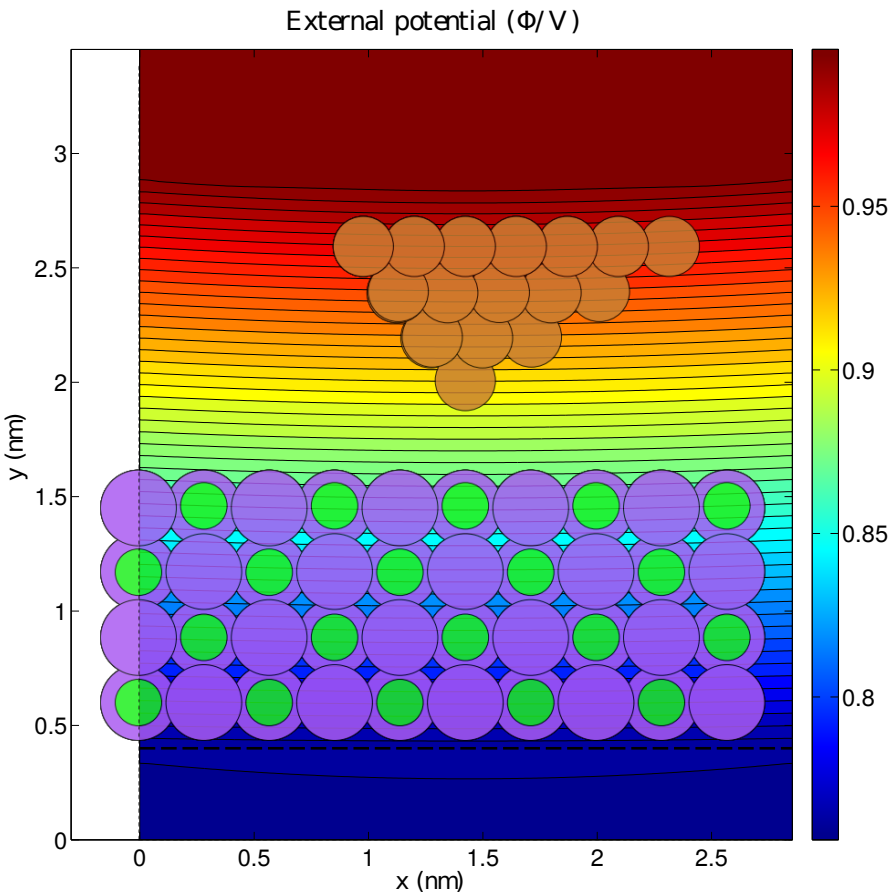


Atomic model



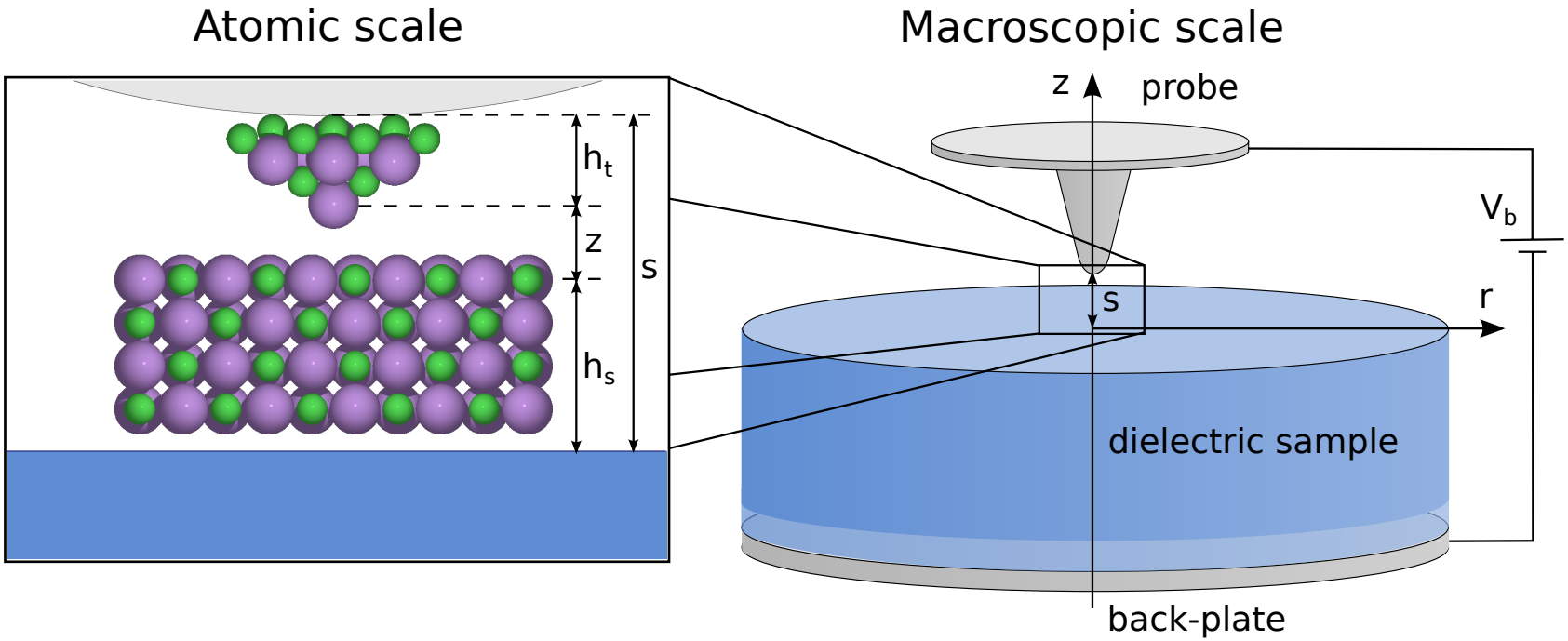
- Solve the electron density distribution using density functional theory (DFT)
- Leads to many quantities of the system, including total energy $\rightarrow$ force on tip

DFT with external potential



- The electrostatic potential is applied to the atomic scale DFT calculation
- The axisymmetric solution is interpolated to a 3D grid that fills the DFT unit cell
- No uniform electric field approximation

Summary of the method



Microscopic force:

$$F_\mu(x,y,z,V) = a(x,y,z)V + b$$

Macroscopic force:

$$F_M(s,V) = \tfrac{1}{2}C'(s)V^2$$