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Simulations of gold surfaces under high electric fields

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Surface defects are thought to play an important role in vacuum breakdowns. Possible nanoprotrusions can significantly enhance the electric field, leading to increased field emission, atom evaporation, and eventually arcing. Atomic scale simulations are very useful in studying dislocation behaviour and surface defects. However, the main material of interest, copper, is in practice covered by an oxide layer, which complicates the simulations. Gold, which also exhibits similar surface behaviour as copper in experiments, is free of this concern and studying it could provide insights into the general processes leading to a breakdown event.
We use a Kinetic Monte Carlo (KMC) method combined with Molecular Dynamics (MD) to simulate diffusion and relaxation processes on the gold surface. To characterize the diffusion of surface adatoms, we have developed an improved migration barrier calculation method. This tethered Nudged Elastic Band (NEB) method is better at describing unstable atomic configurations, which occur frequently around surface defects. We use the MD simulations, as well as KMC with tethered NEB, to study defect formation and stability on gold surfaces under high external electric fields.

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Modelling and Simulations

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