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# Diffusion on Cu surface under Electric Field with Collective Variable -accelerated Molecular Dynamics

## Introduction

Vacuum arc breakdowns can hinder the operation of high voltage devices such as the Compact Linear Collider (CLIC). Surface diffusion is one of the phenomena proposed to play a role in the formation of vacuum arcs.

Our goal is to simulate diffusion on the Cu surface with Molecular Dynamics (MD). Electric field is not a standard component of MD; we have used an external FEM field solver developed in our group: Femocs.

As diffusion is a much slower process than thermal atomic motion, we have accelerated MD with Collective Variable -driven Hyperdynamics (CVHD).

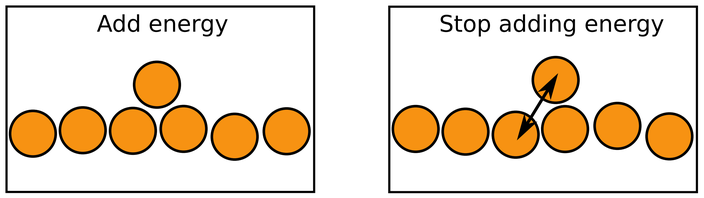
## Conclusions and Outlook

- CVHD gives up to six-fold acceleration at low temperatures.
- Electric fields appear to promote jumps on top of atomic steps, and to stabilize small protrusions
- Future simulations: growth of larger tips.

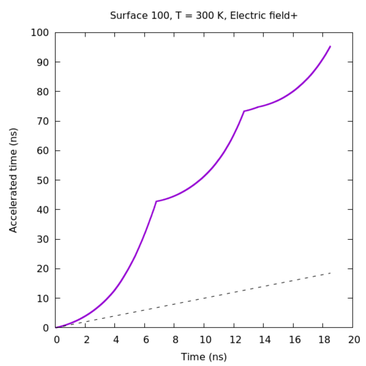
## Collective variable acceleration

Collective Variable -driven Hyperdynamics (CVHD) is an acceleration method that adds artificial energy to the MD system to push it away from potential energy minima.

We defined the collective variable based on the bond lengths in the system. When all bonds are near their equilibrium value, more energy is added to the system.



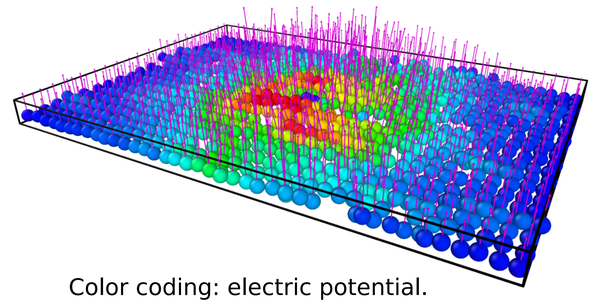

The algorithm stretches the simulation time according to the added energy. Whenever there is a transition, the acceleration is reset.



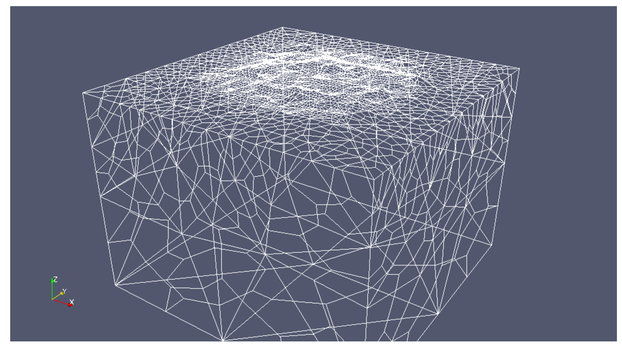

CVHD method: Bal, Kristof M., and Erik C. Neyts. *Journal of chemical theory and computation* **11**.10 (2015): 4545-4554.

## Femocs - electric field solver

Femocs (Finite Elements Methods for Crystal Surfaces) is a program that can solve the electric field, charges, forces, currents, heating and field emission, given atomic coordinates and the value of the external field.



Color coding: electric potential.
Arrows: forces exerted by the electric field.



The mesh generated by Femocs based on atomic coordinates

Femocs: Veske, Mihkel, et al. *Journal of Computational Physics* **367** (2018): 279-294.

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