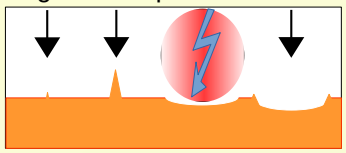
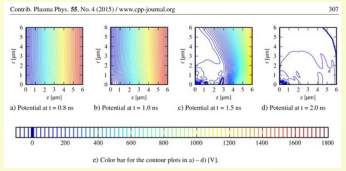
Jyri Kimari[1], Ye Wang[2], Andreas Kyritsakis[2], Ekaterina Baibuz[1], Veronika Zadin[2], Flyura Djurabekova[1]

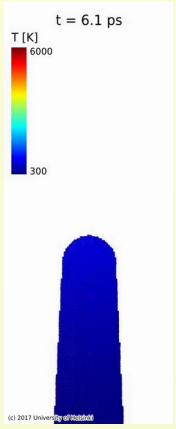
[1]Helsinki Institute of Physics and Department of Physics, University of Helsinki, Finland
[2]Institute of Technology, University of Tartu, Estonia

Field enhancer sharpening mechanism via biased surface diffusion

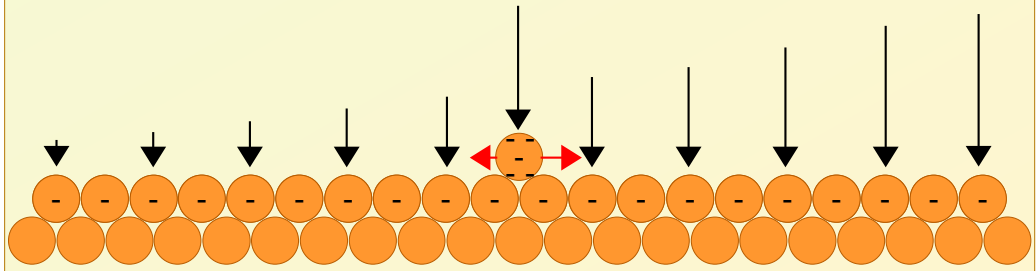
Breakdown mechanism on Cu surface.
Sharpening of initial protrusions lead to runaway?





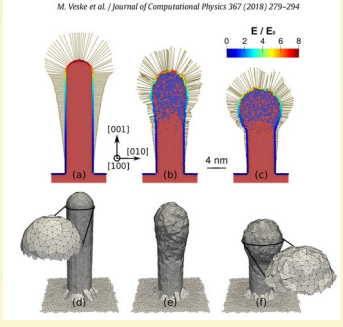


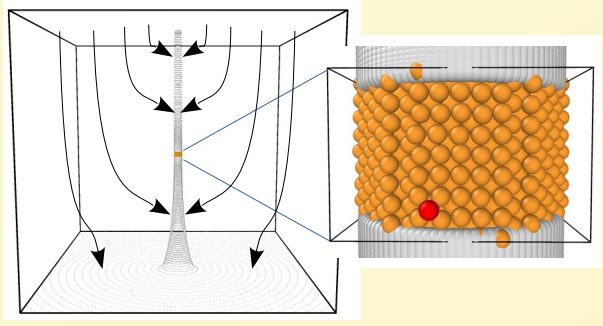
Theory: electric field gradient biases diffusion



$$\Delta E_m \propto \mathcal{M}\,\gamma + \mathcal{A}\,\gamma F$$

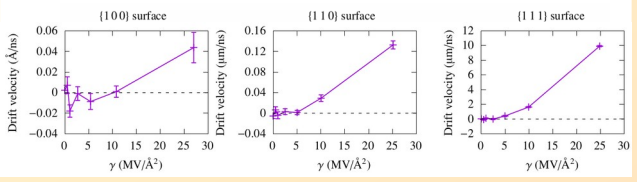
Molecular dynamics simulations with E field



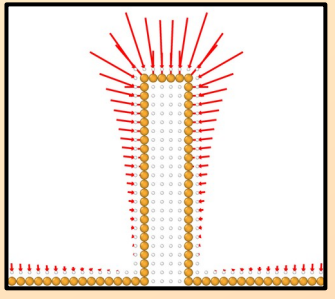


MD coupled with finite elements method Laplace equation solver

Result: Diffusion bias agrees with theory & DFT



Surface	$\mathcal{M}$ (eÅ)		$\mathcal{A}$ (eÅ²/V)	
	MD	DFT	MD	DFT
Cu {100}	2 ± 1	0.106 ± 0.003	0.0 ± 0.5	0.27 ± 0.02
Cu {110}	0.7 ± 0.1	0.094 ± 0.006	**0.24 ± 0.08**	**0.30 ± 0.04**
Cu {111}	0.61 ± 0.06	0.162 ± 0.003	**0.27 ± 0.05**	**0.23 ± 0.02**



Field enhancers facet and sharpen

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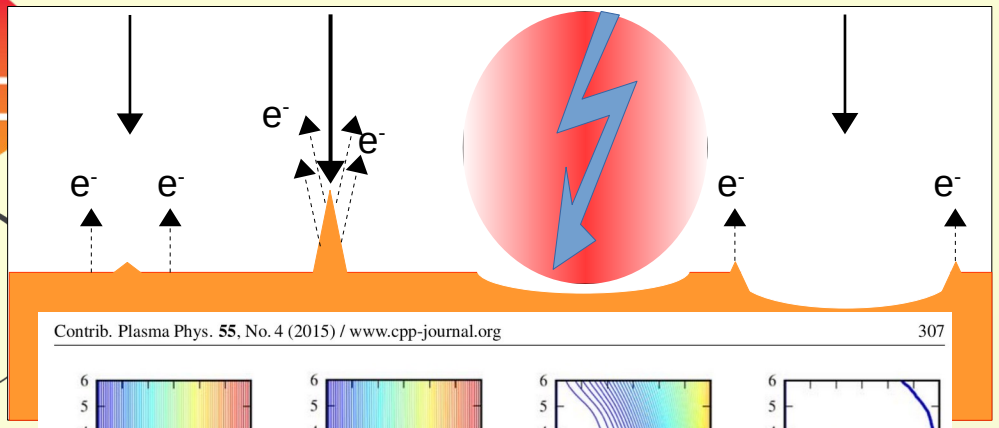
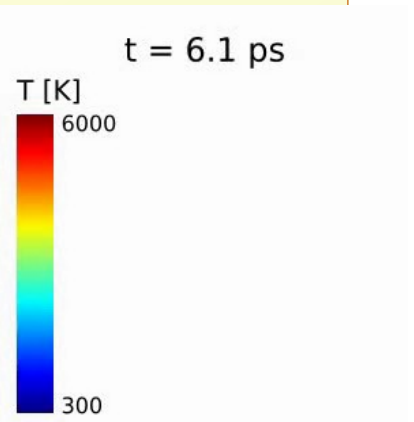
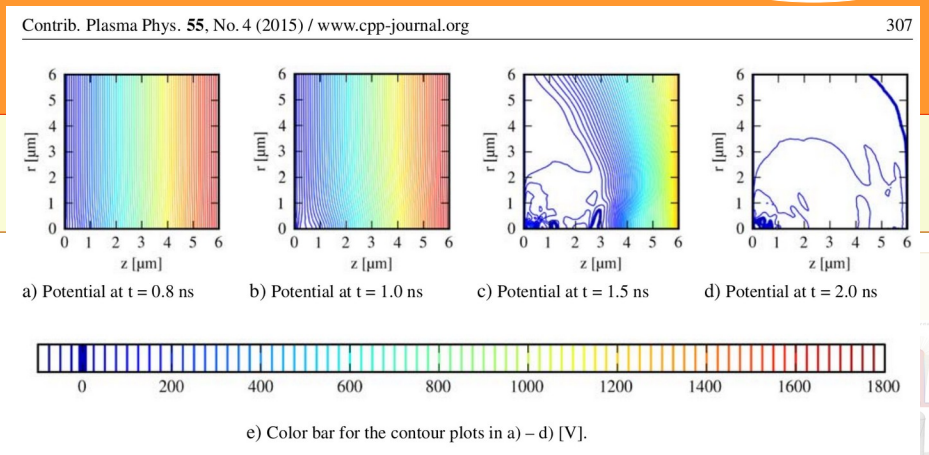
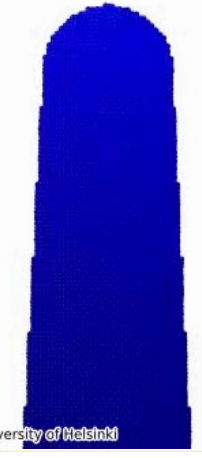






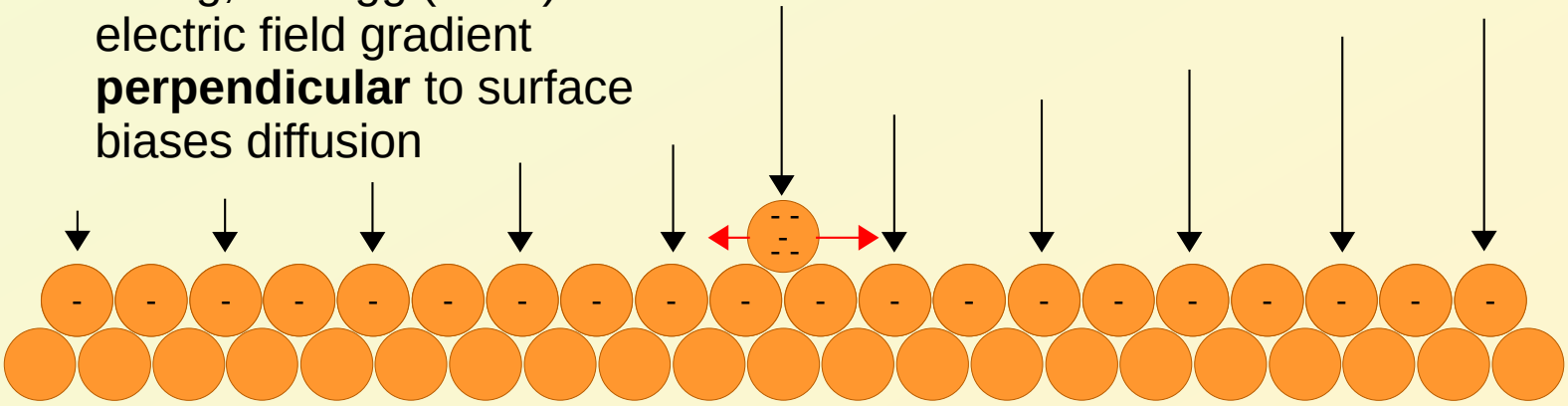


A. Kyritsakis et al. *Journal of Physics D: Applied Physics* 51.**22** (2018):225203.

Timko, Helga, et al. *Contributions to Plasma Physics* **55**.4 (2015): 299-314.

Theory: electric field gradient biases diffusion

Tsong, Kellogg (1975):
electric field gradient
perpendicular to surface
biases diffusion



Change in migration energy barrier: $\Delta E_{\mathrm{m}} \propto \mathcal{M}\ \gamma + \mathcal{A}\ \gamma F$

dipole moment polarizability

F = electric field
γ = electric field gradient

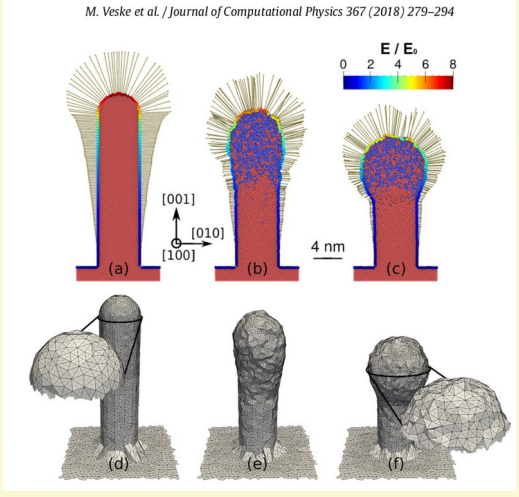
A. Kyritsakis et al. *Physical Review B* 99.**20** (2019): 205418

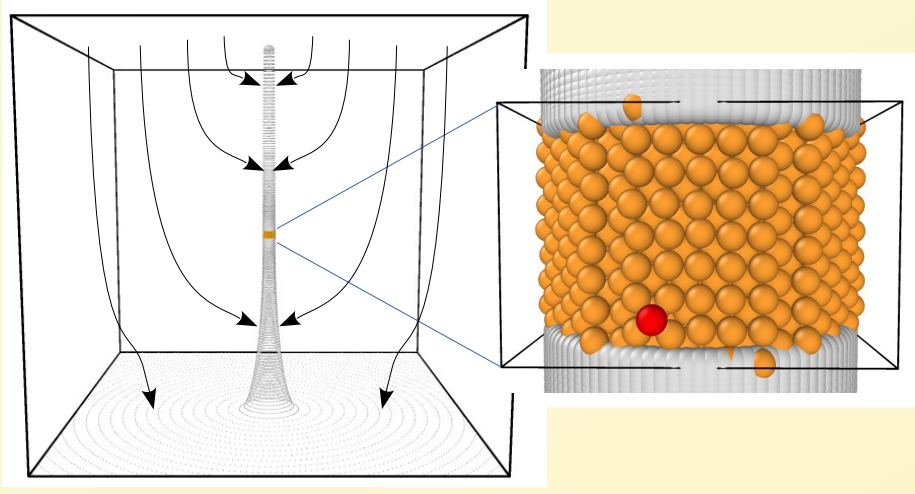
Field enhancer sharpening

Simulations

Results

Molecular dynamics simulations with E field





MD coupled with finite elements method Laplace equation solver

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

Kimari, Jyri, et al. In preparation.

{100} surface accelerated with collective variable hyperdynamics (CVHD)

K. M. Bal and E. C. Neyts. *Journal of chemical theory and Computation* **11**.10 (2015): 4545–4554

Field enhancer sharpening

Theory

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dipole moment — polarizability

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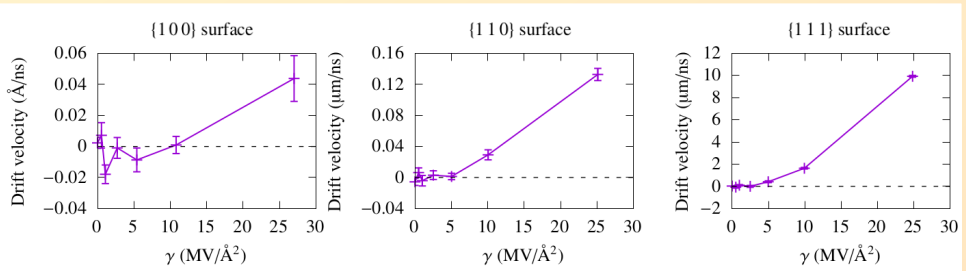

"Drift velocity" ~ bias as function of gradient

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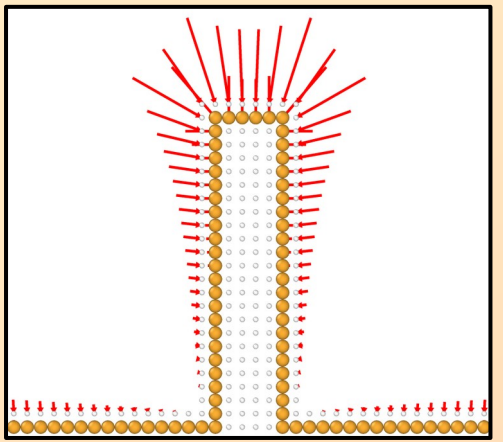
Electric properties sanity check from DFT



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