Stability of thin nanotips under high electric field

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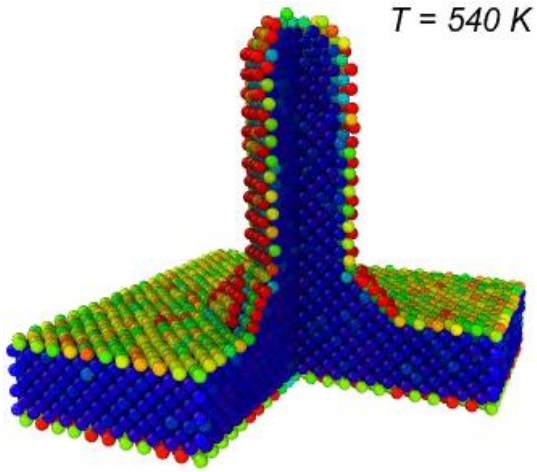
Outline

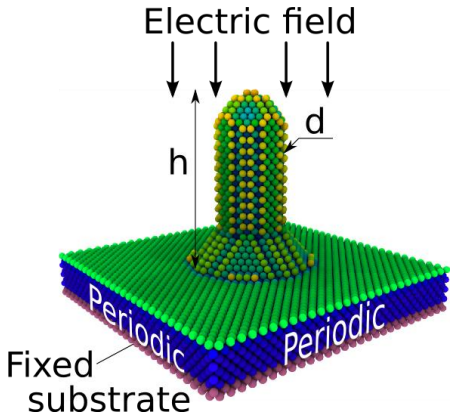
- <100> to <110> reorientation
- Shape memory effect
- Determining the critical temperature
- Electric field as stabilizer and destabilizer
- The change of stability range due to the electric field

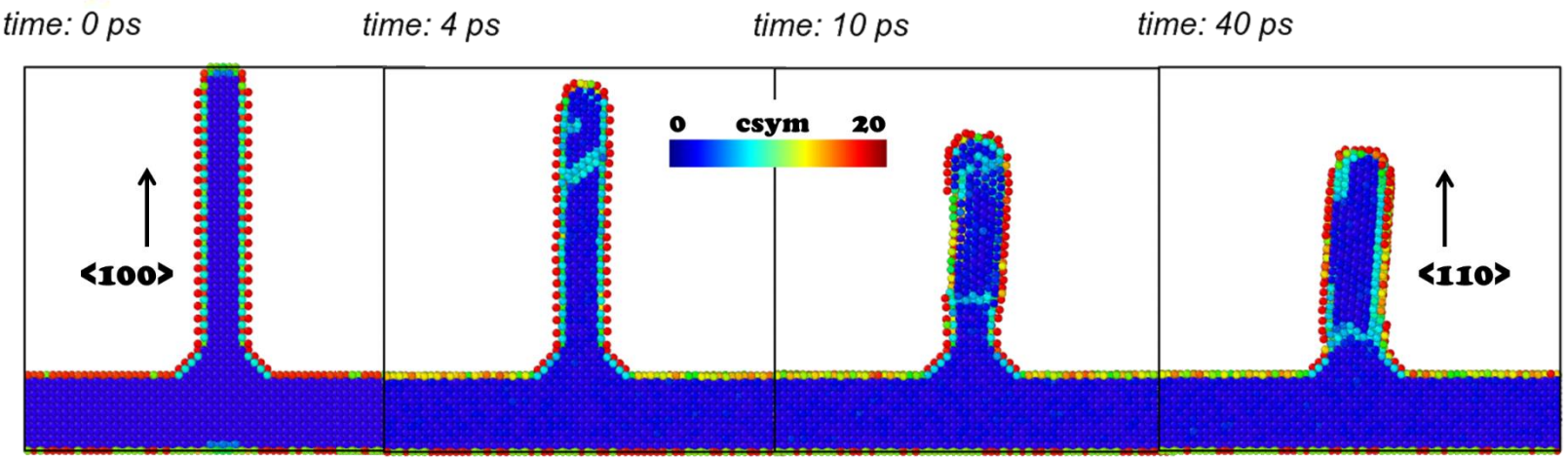
<100> → <110> reorientation

- Reorientation occurs if T > Tcr
  - Shape memory effect
- h = h(T) → Tcr = Tcr(E)
  - Does high E stabilize tip?

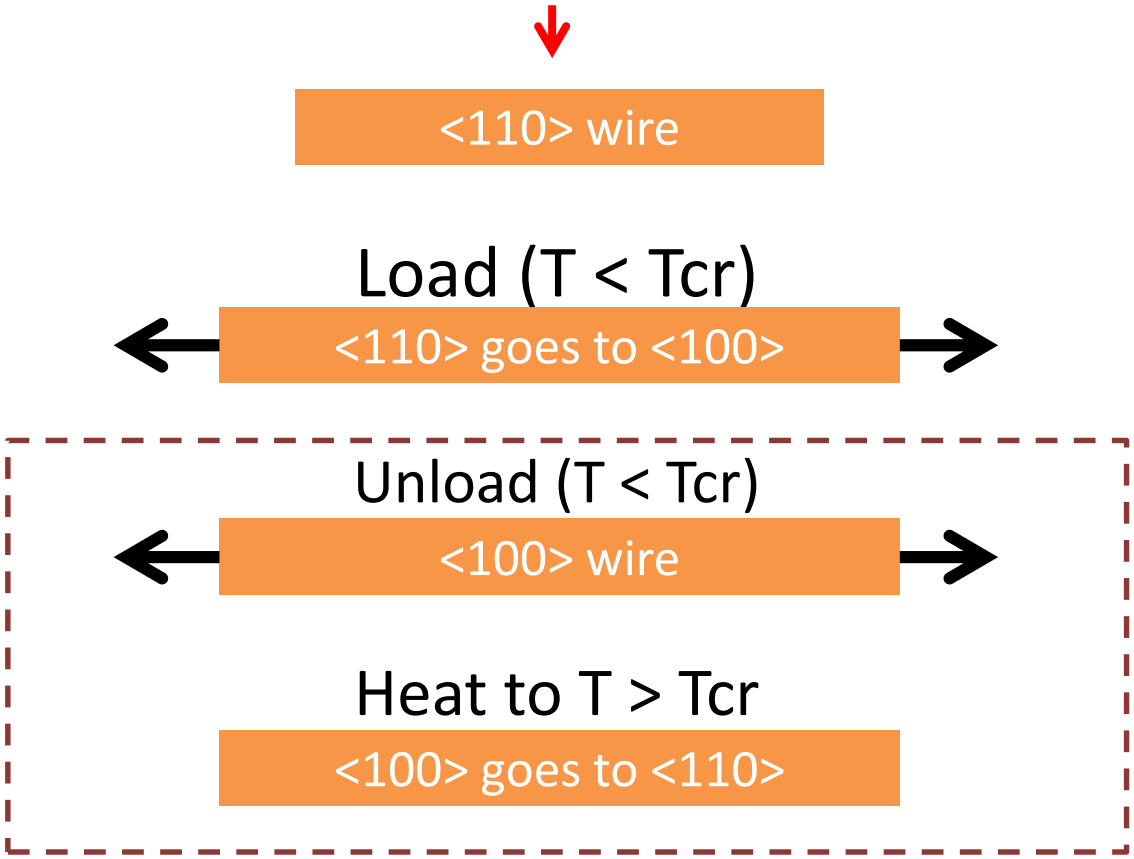
E = 0-1.5 GV/m
T ramp rate = 1 K/ps
h = 6-18 nm, d = 2-2.8 nm







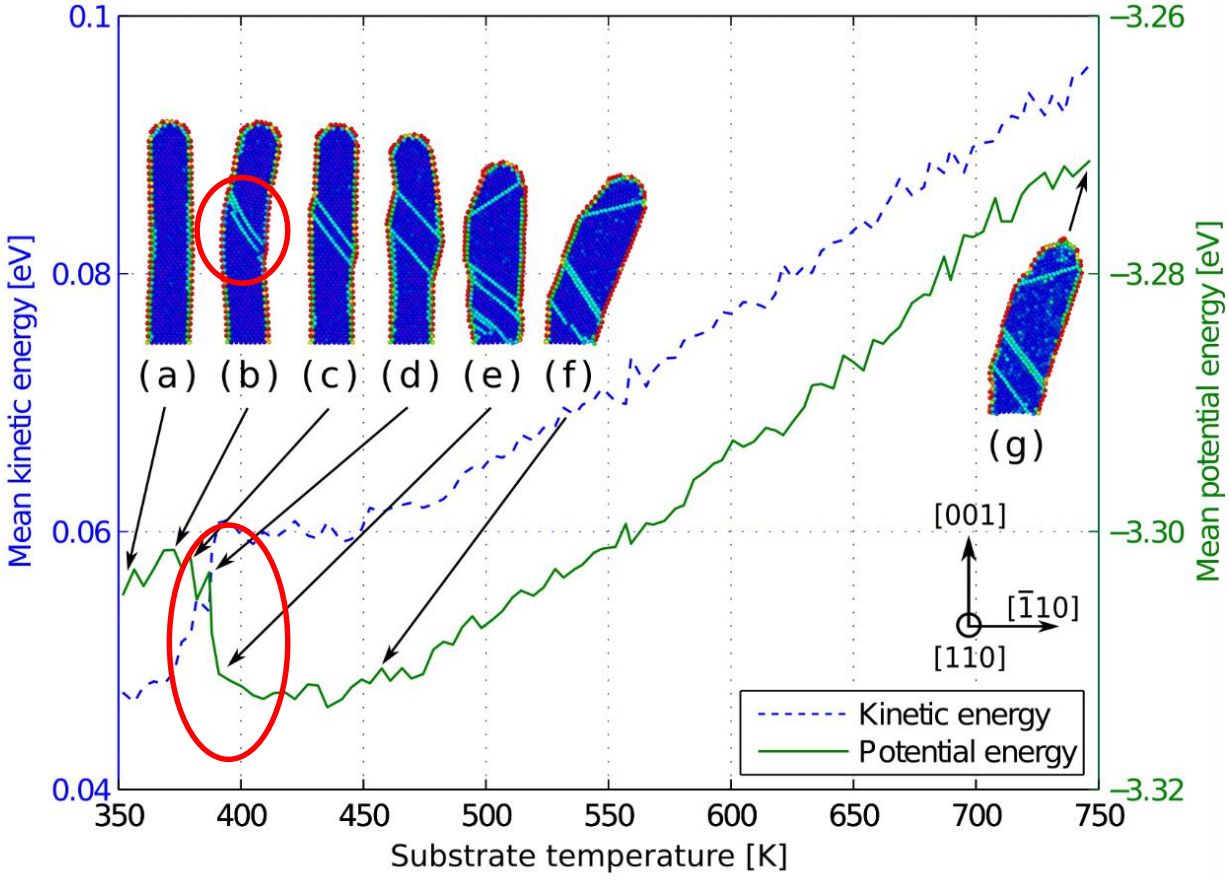
Shape memory effect



Determining critical temperature

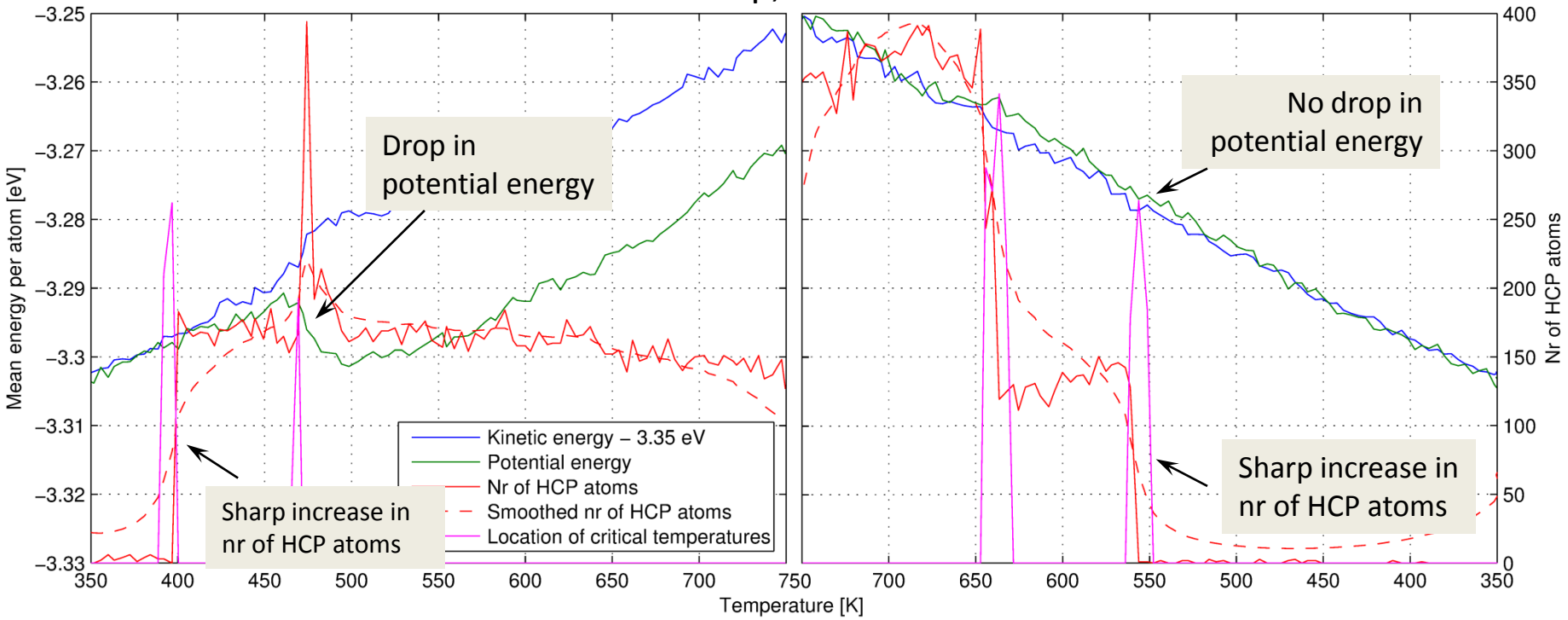
a) Scan for the change of potential energy

b) Scan for the dislocations / nr of HCP atoms



Determining critical temperature

The same simulation setup, different initial atomic velocities



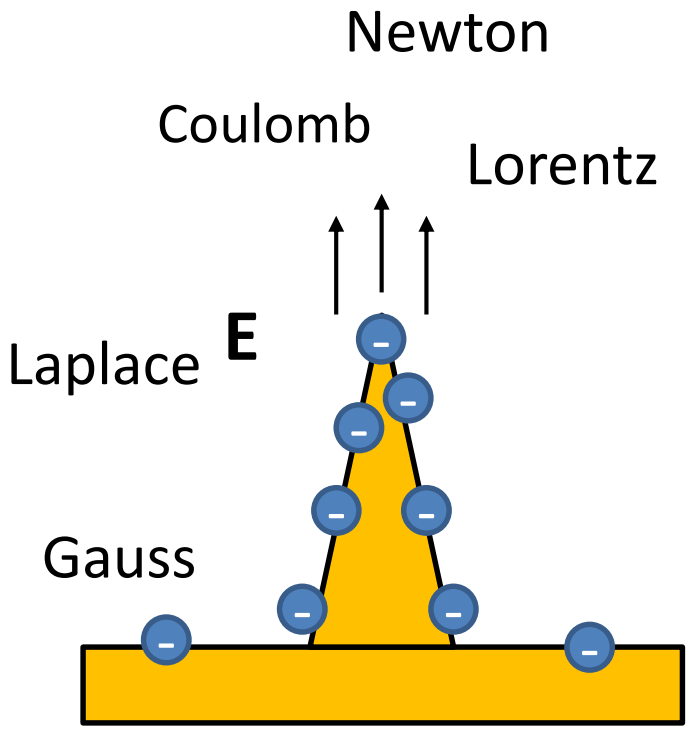
- Scan of potential energy doesn't always reveal the T_{cr},
- Scan of nr of HCP atoms does,
- Thermal separation between the methods 0 – 30 K

Electric field as (de-)stabilizer

Stabilizer

- E induces surface charge
- σ pulls protrusion up
- More T needed to collapse the tip

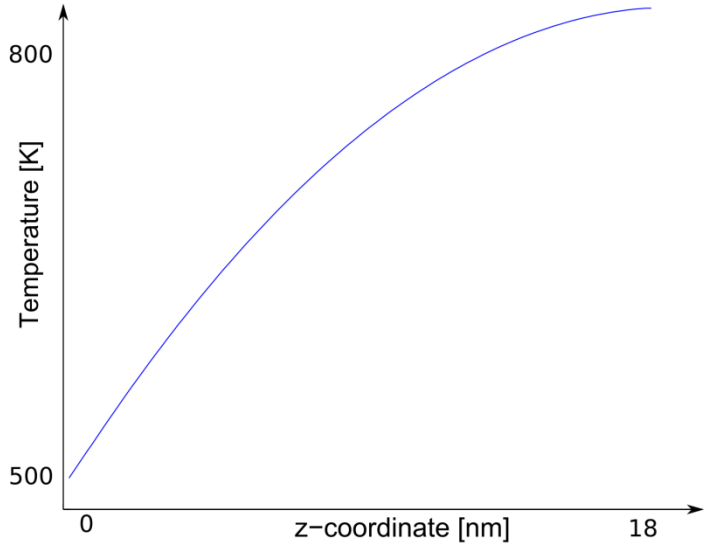
Hybrid Electrodynamics – Molecular Dynamics code HELMOD

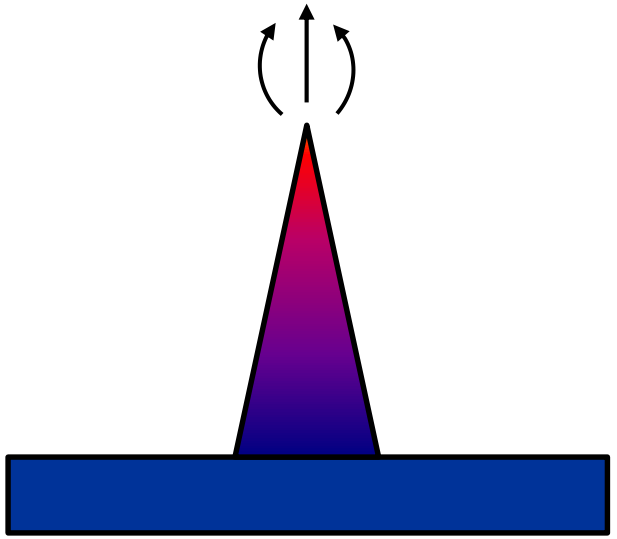


Electric field as (de-)stabilizer

Destabilizer

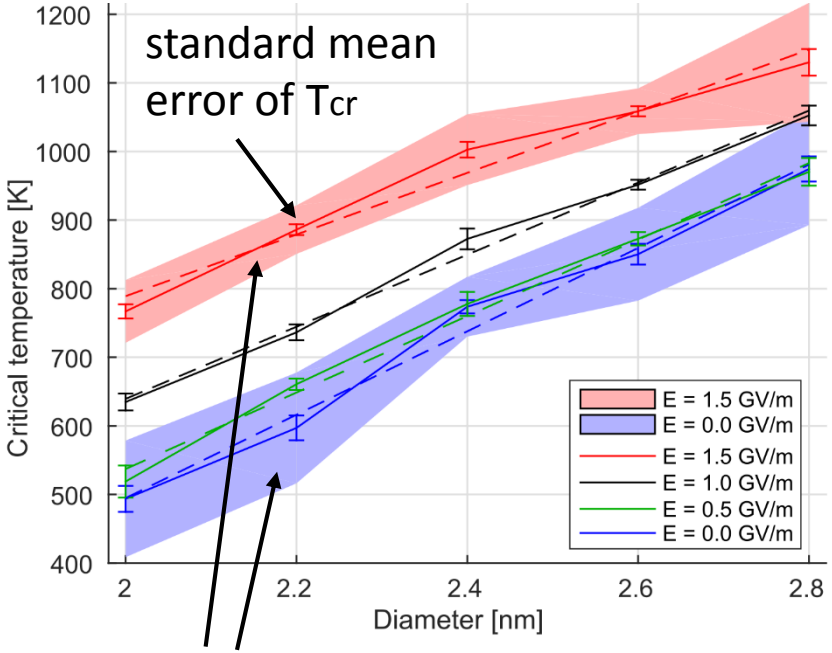
- E induces field emission currents
- Joule heating & electromigration cause non-uniform temperature distribution
- Less additional heat needed to collapse the tip
- Big cold + small hot = cooler average



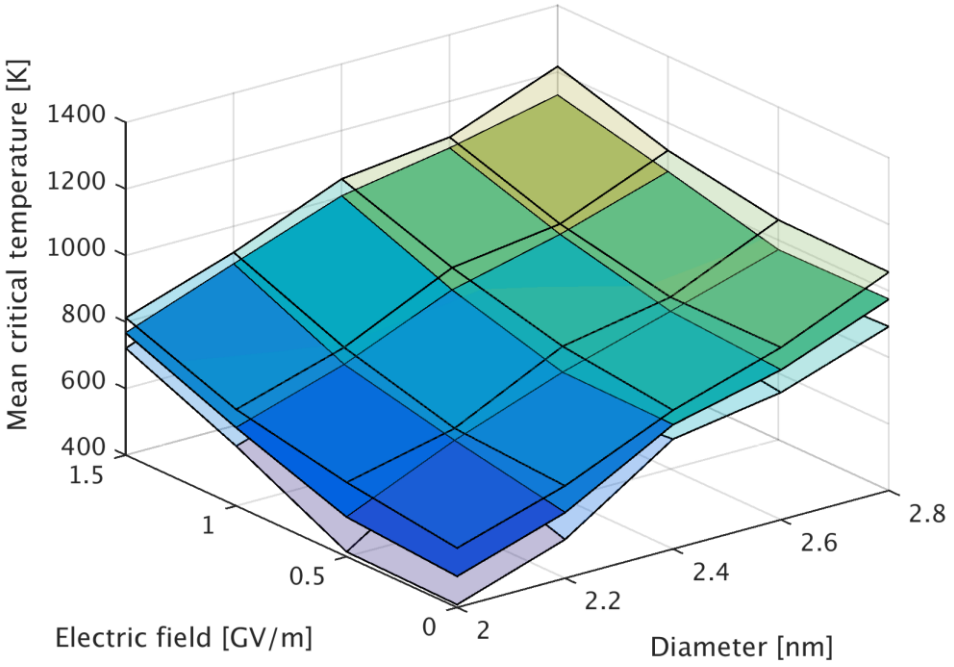


Results

Electric field as stabilizer



1 standard deviation of T_{cr}

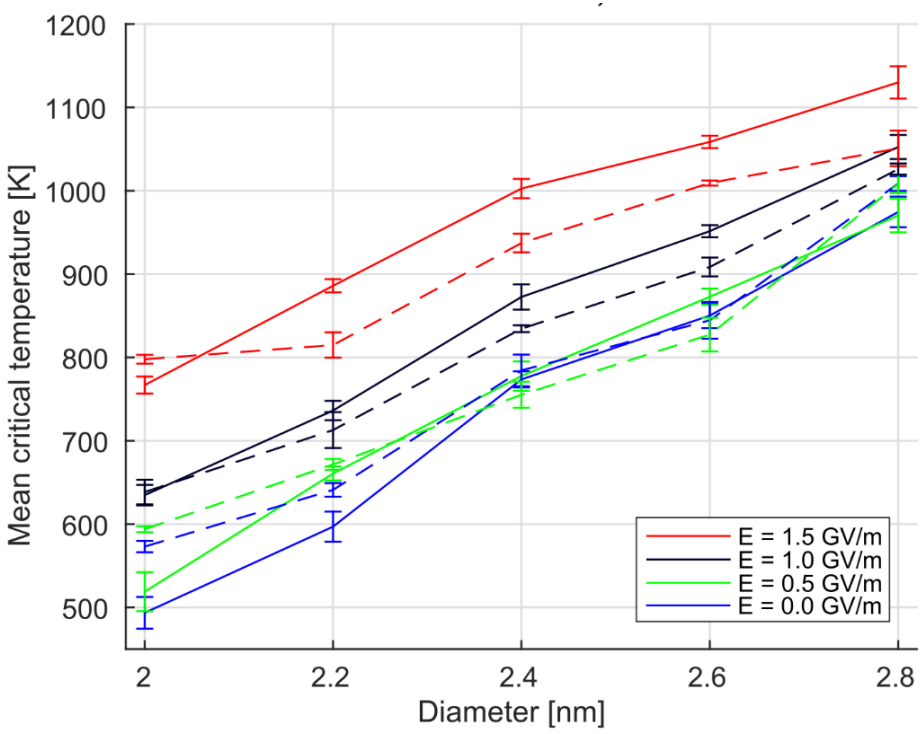


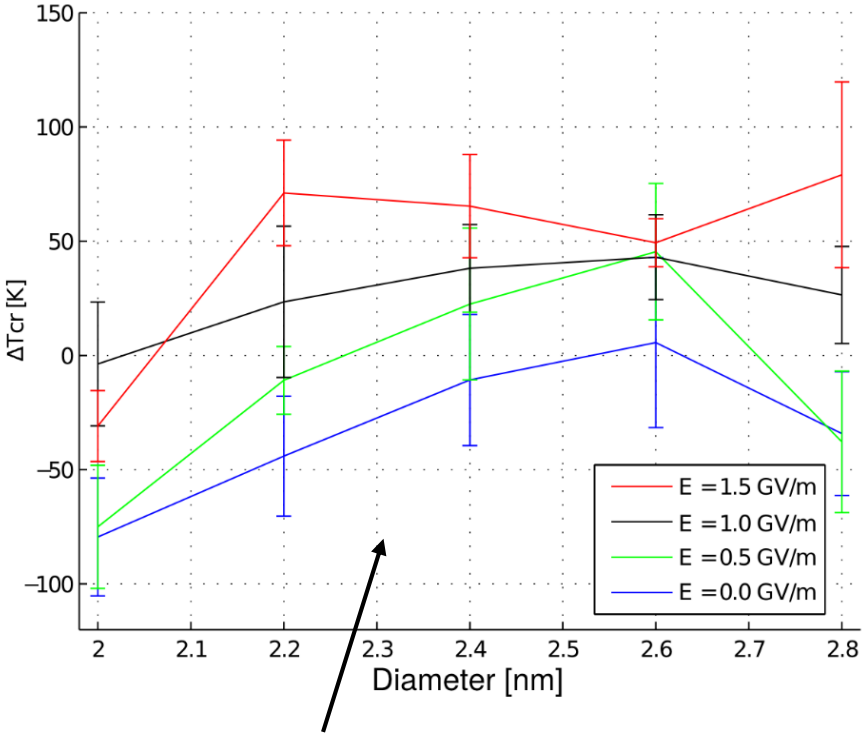
Solid line – mean critical temperature
Dashed line – its linear fit

Middle plane – mean critical temperature
Upper & lower plane – its standard mean error

Results

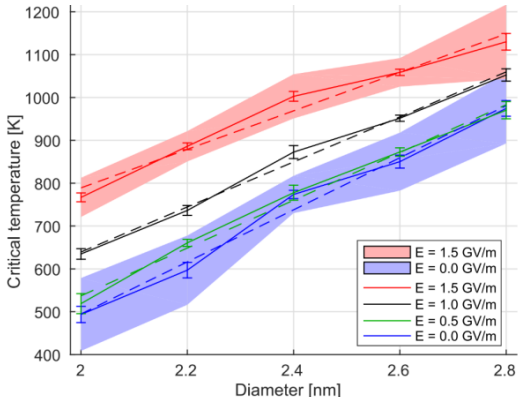
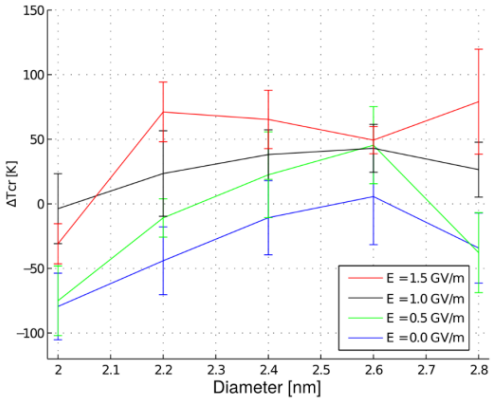
Electric field as destabilizer





Solid line – electric field ON, field current OFF
Dashed line – electric field & field current ON

Difference of Tcr(FME on) and Tcr(FME off)

Conclusions

- <100> Cu nanoprotrusions with d < 2.8 nm reorient / collapse into <110> if T > T_{cr}
- Tensile stress from electric field increases the T_{cr} hundreds of kelvins
- Field emission current lowers the T_{cr} tens of kelvins