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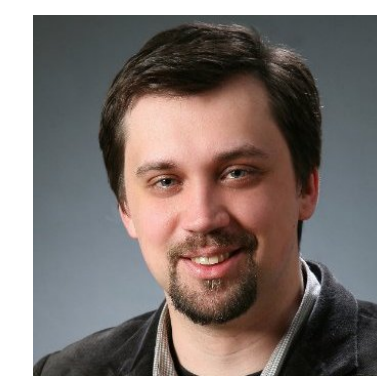
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Growth mechanism of a nano-protrusion on a tungsten tip under electric field

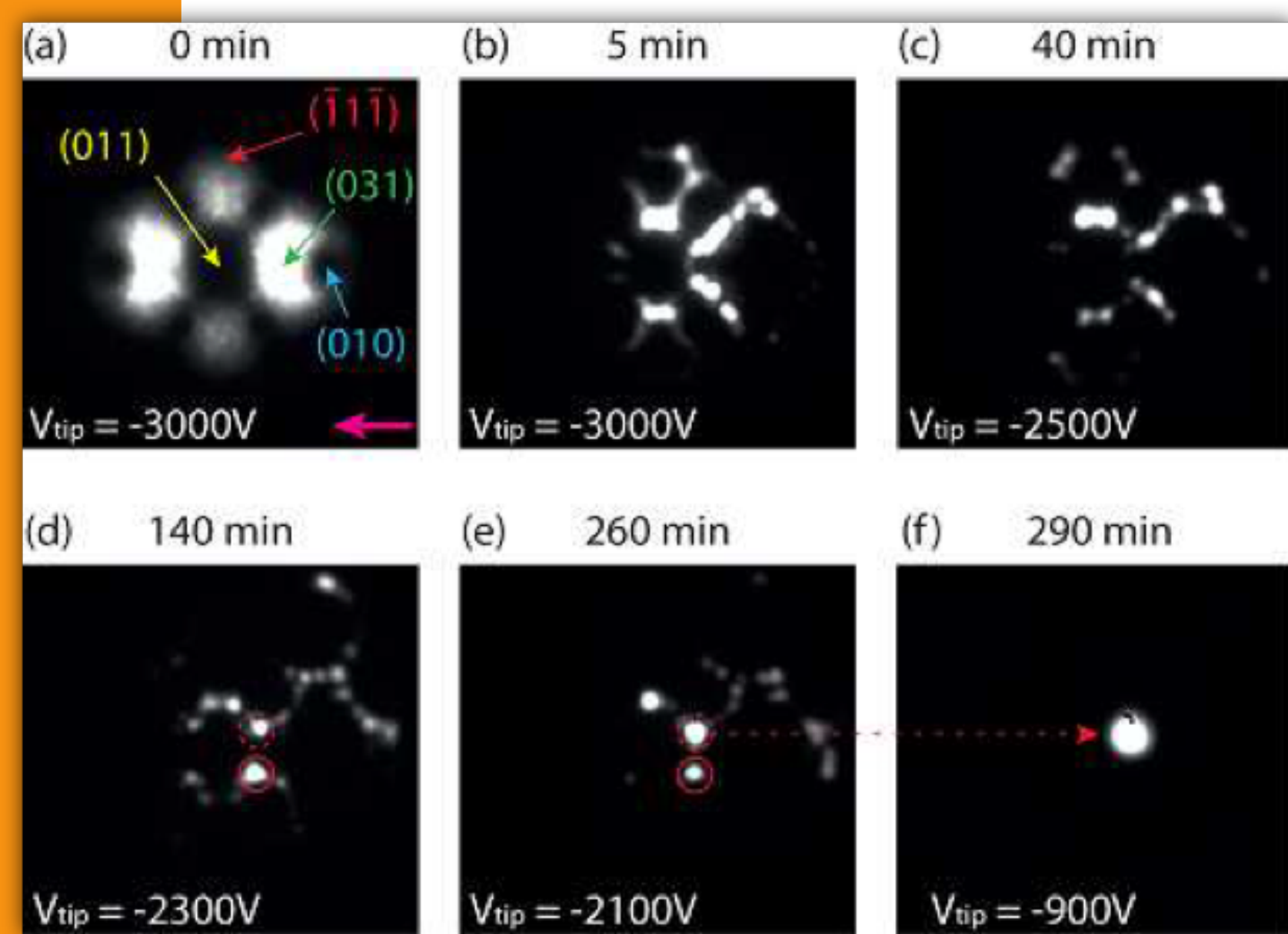
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Abstract

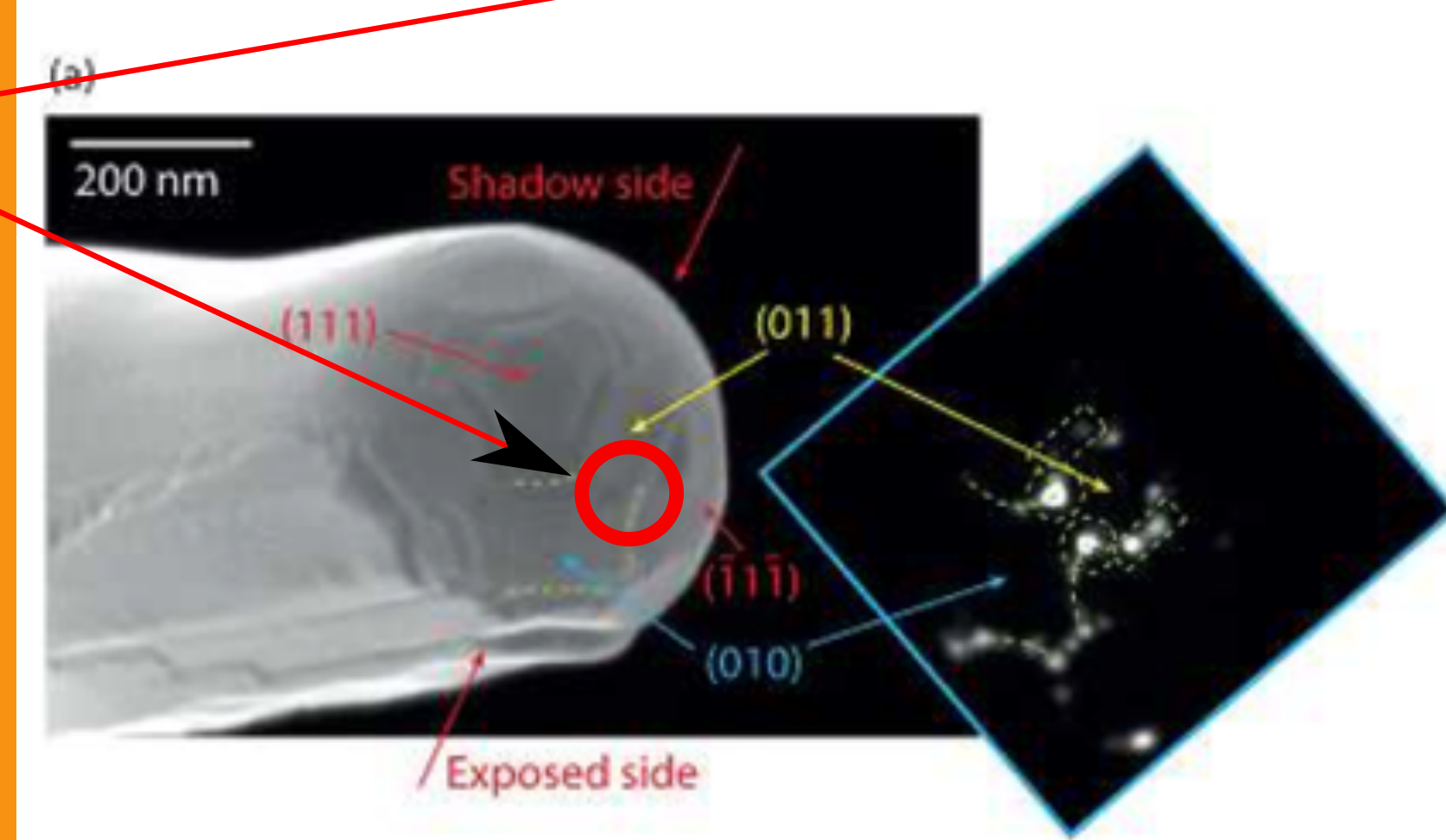
Recent experiments showed that femtosecond laser irradiation of a sharp 250 nm tungsten tip exposed to strong DC electric field leads to gradual and reproducible surface modifications. Asymmetric surface faceting mainly on the laser-exposed side along with the formation of a few nanometers high nano-protrusion in the corner between the facets were observed. In this work, we investigate how laser pulses along with the field emission conditions change the properties of a 250 nm tungsten tip. We also used a KMC model to simulate a growth of nano-protrusions on a faceted surface of W.

Field emission images of the 250 nm radius tungsten tip irradiated by the laser for 290 minutes indicate the formation of the nanotip



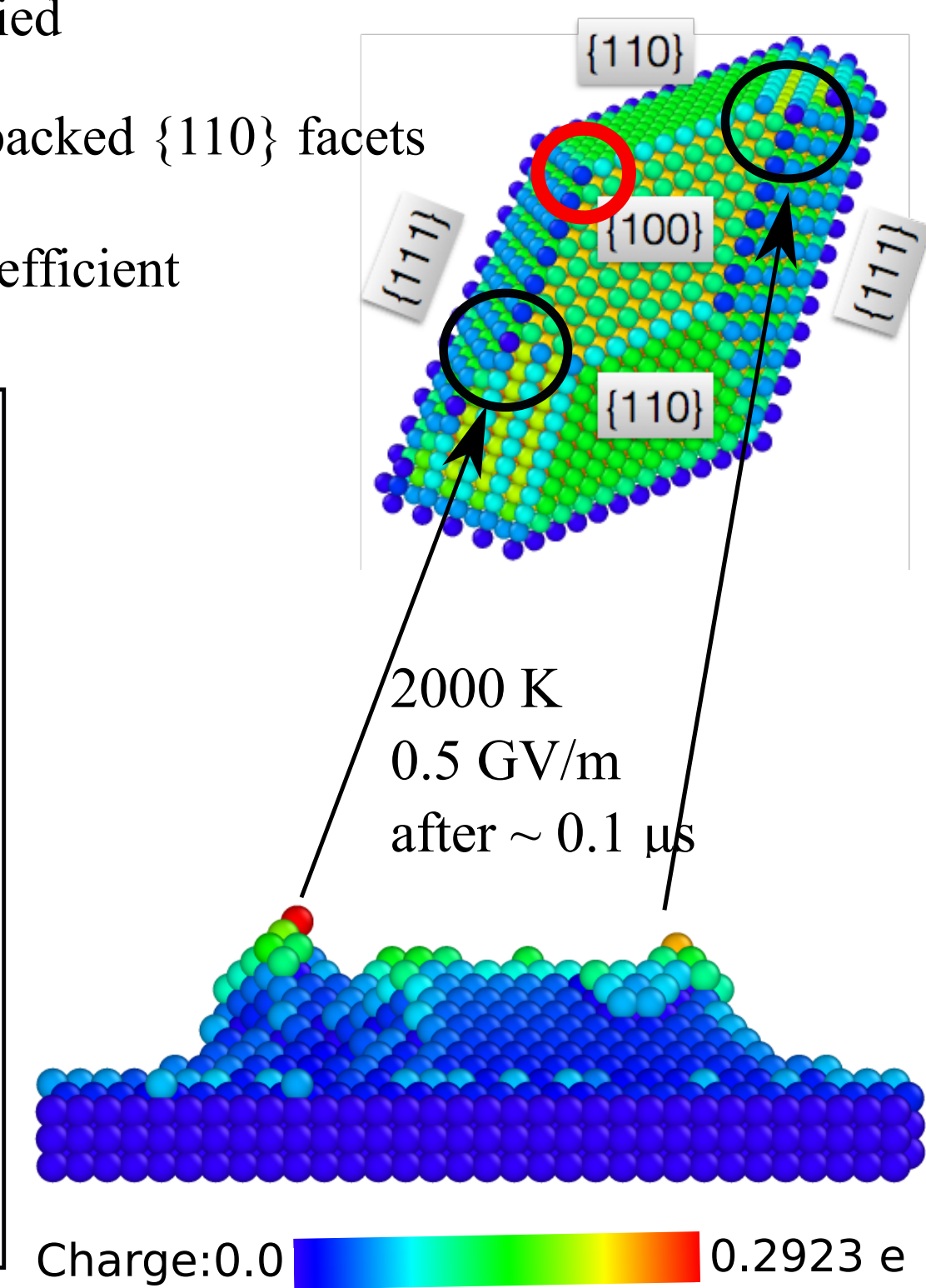
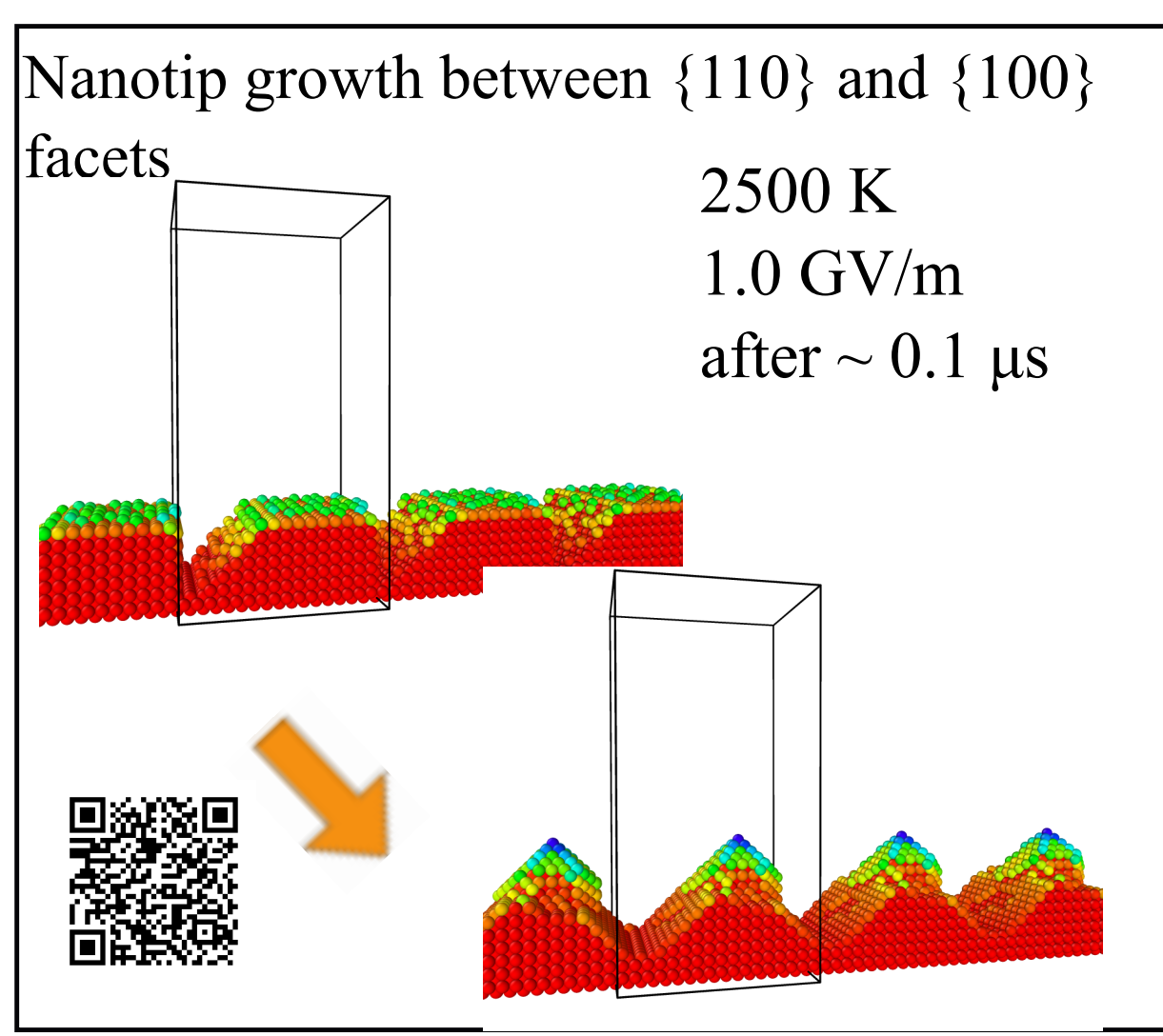
H. Yanagisawa, et al. APL Photonics (2016)

Ultrafast sub-fs laser pulses and field emission conditions result in the growth of a nanotip



Preliminary KMC results

- Small plateau of the size ~ 8 nm was studied
- Plateau reorganised into ridges of close packed $\{110\}$ facets
- Larger system will be studied with more efficient FEMOCS electric field solver



KMC code *Kimocs*

V. Jansson, E. Baibuz, F. Djurabekova, Nanotechnology (2016)

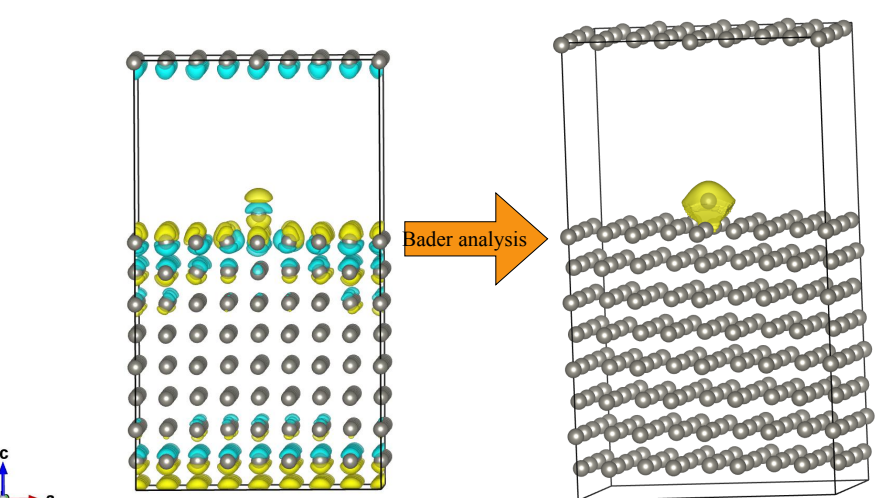
- Rigid lattice is assumed
- Thermally activated jumps to vacant 1nn sites

$$\Gamma = \nu e^{-\frac{E_m}{k_B T}}$$

where ν is the attempt frequency, k_B - Boltzmann's constant, T - the temperature, and E_m - the migration barrier that an atom needs to overcome in order to make a jump.

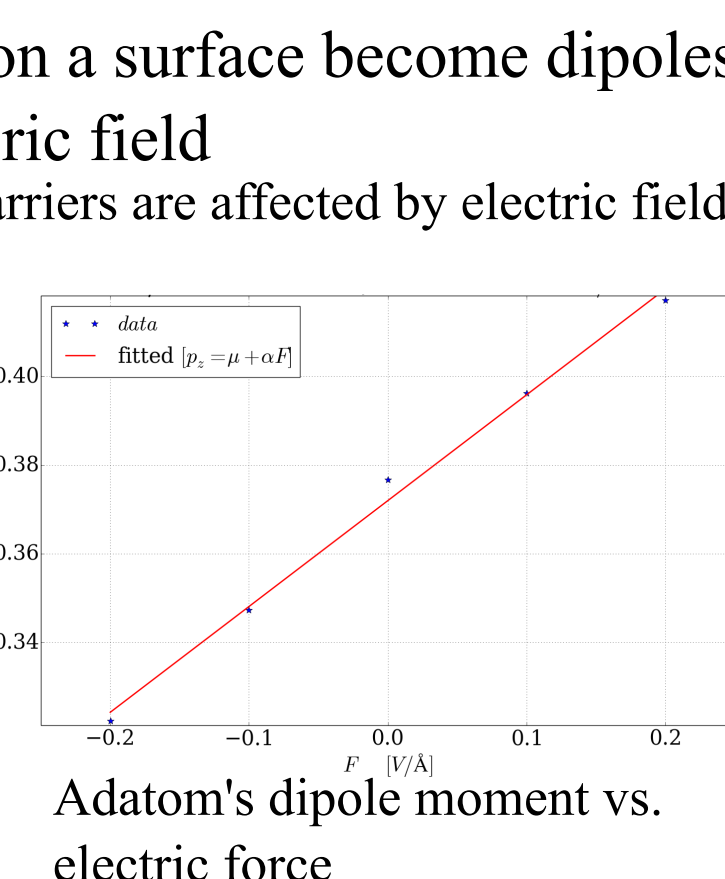
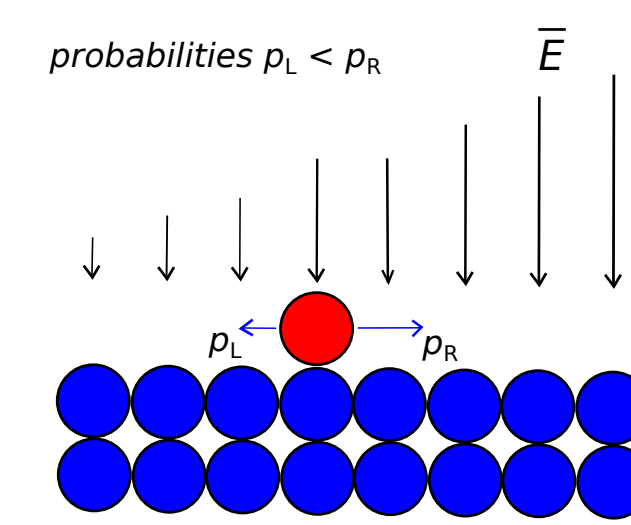
- Adatoms on a surface become dipoles under electric field
- Migration barriers are affected by electric field

W adatom on W surface. DFT study

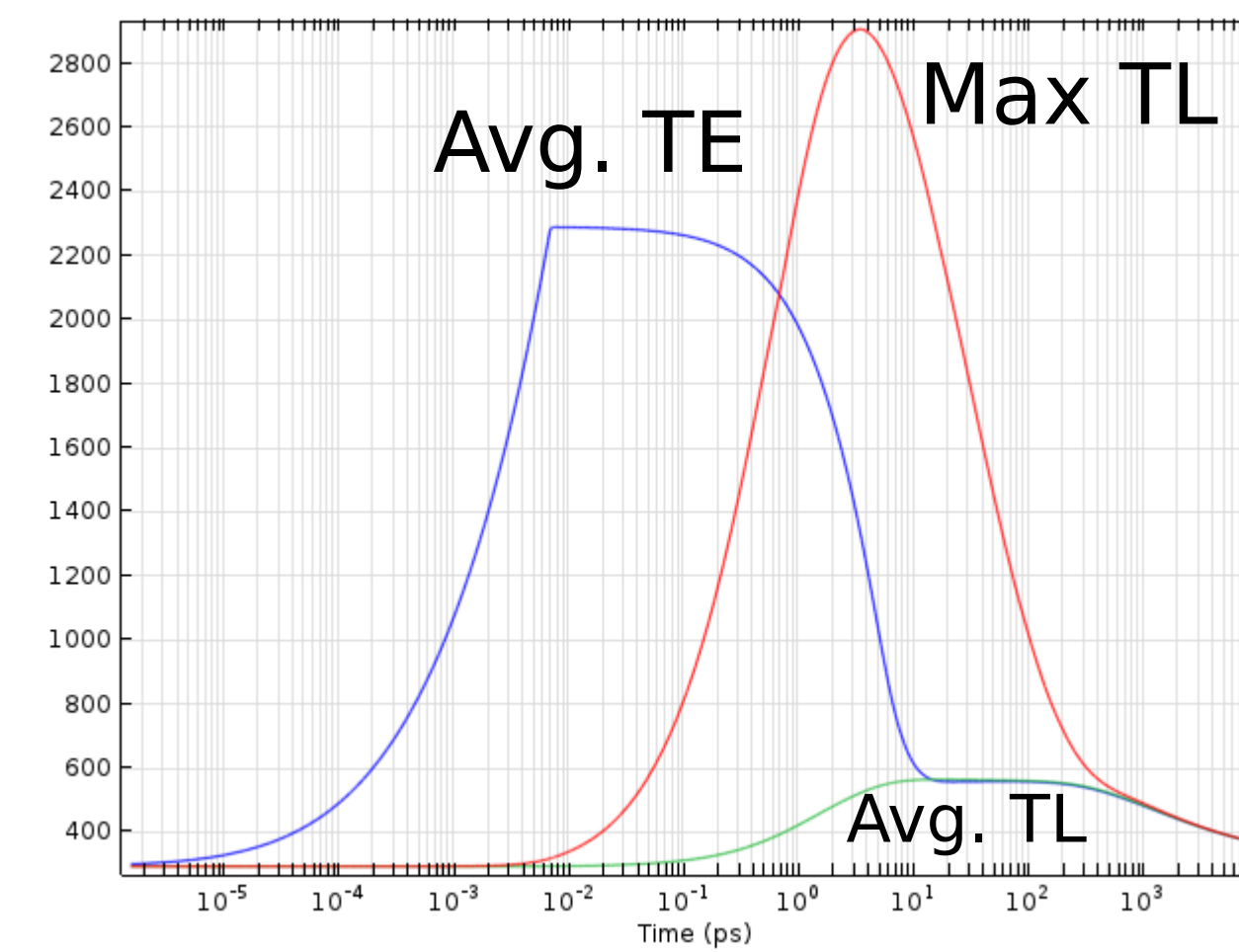


Charge density introduced by electric field on a slab with an adatom

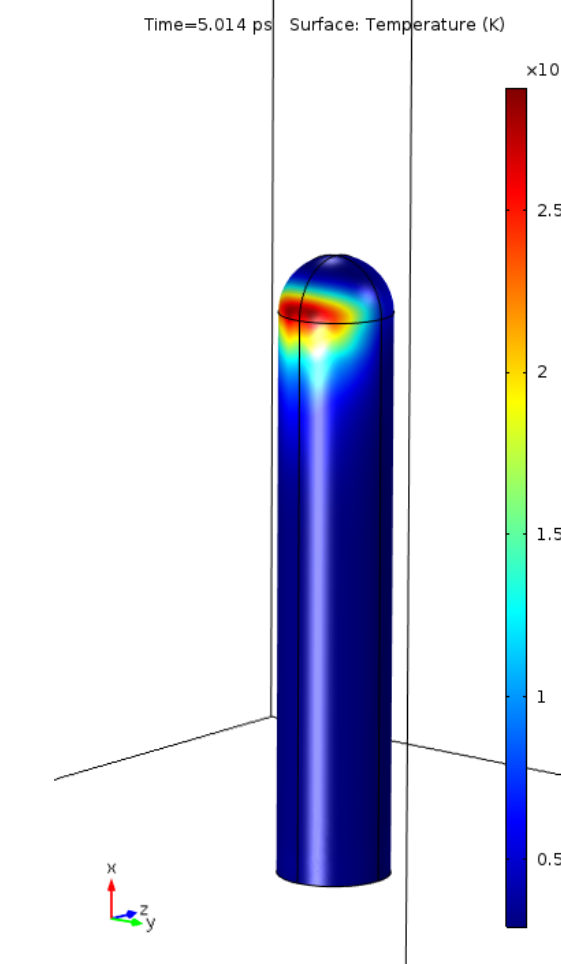
- Accumulation of electrons by electric field
- Depletion



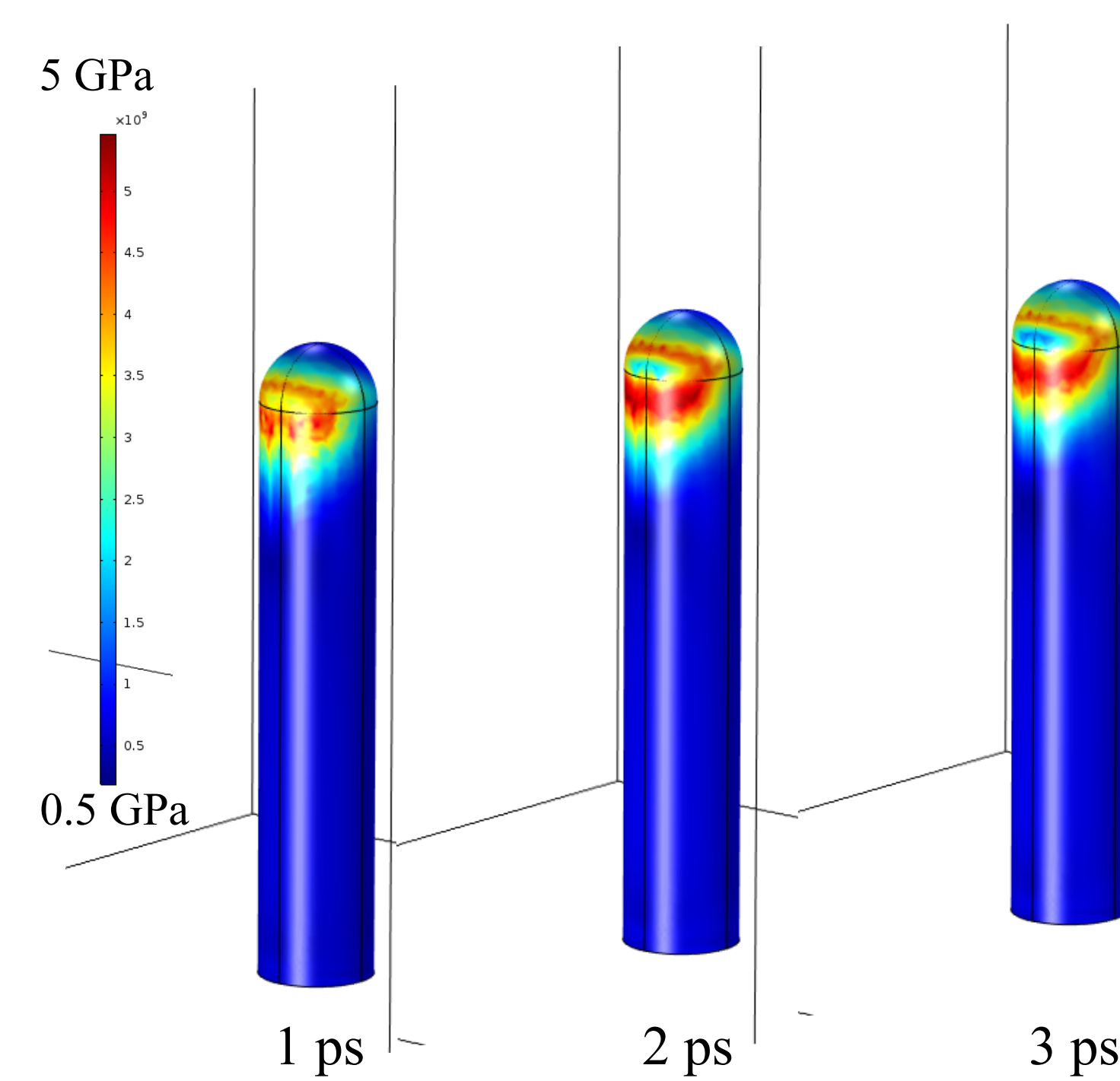
FEM study



Temperature behaviour after the laser impulse; TL denoting lattice temperature, TE electronic temperature. Lattice temperature does not reach melting temperature in the current model



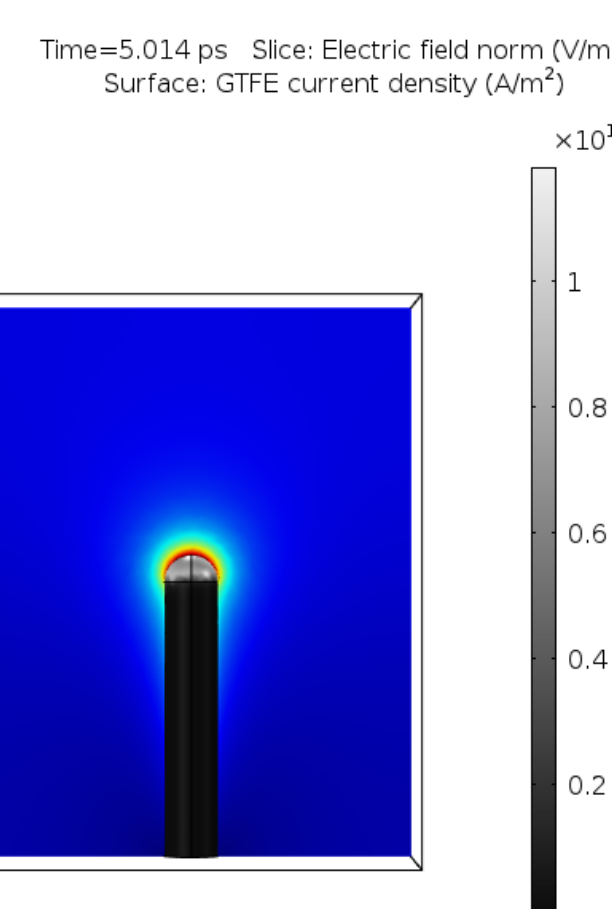
Lattice temperature distribution at 5 ps, near lattice temperature peak



A Von Mises stress wave can be observed as energy is transferred to the lattice
T=0 is taken as start of the laser impulse

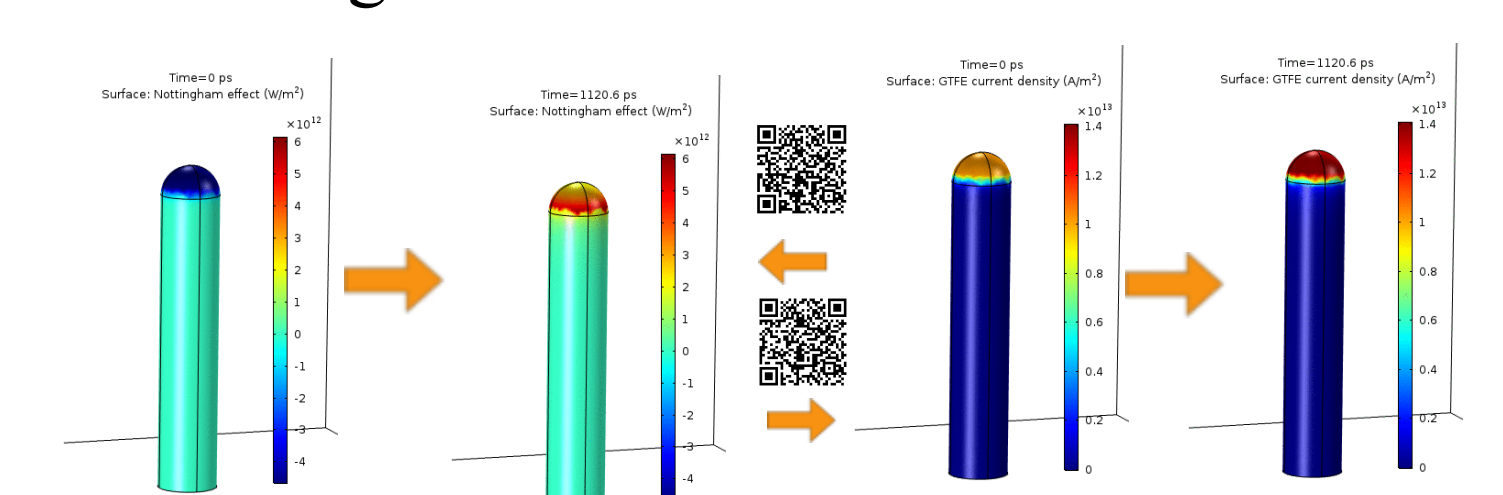
- Two temperature model was used
- Laser pulse heats up the electrons
- The atomic lattice is heated up by electron-phonon coupling with a delay
- Laser heating creates massive thermal stresses.

FEM study extended with emission currents

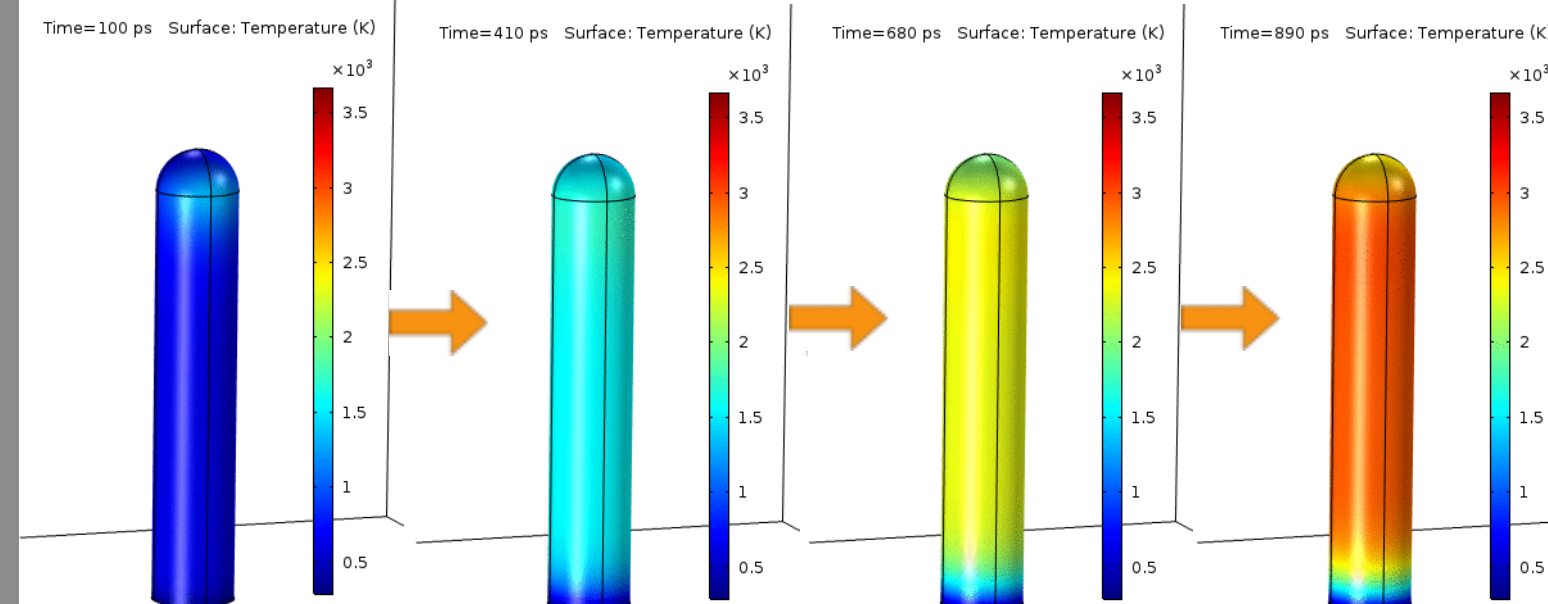


The electric field norm at the tip apex is taken to be ~ 17 GV/m.

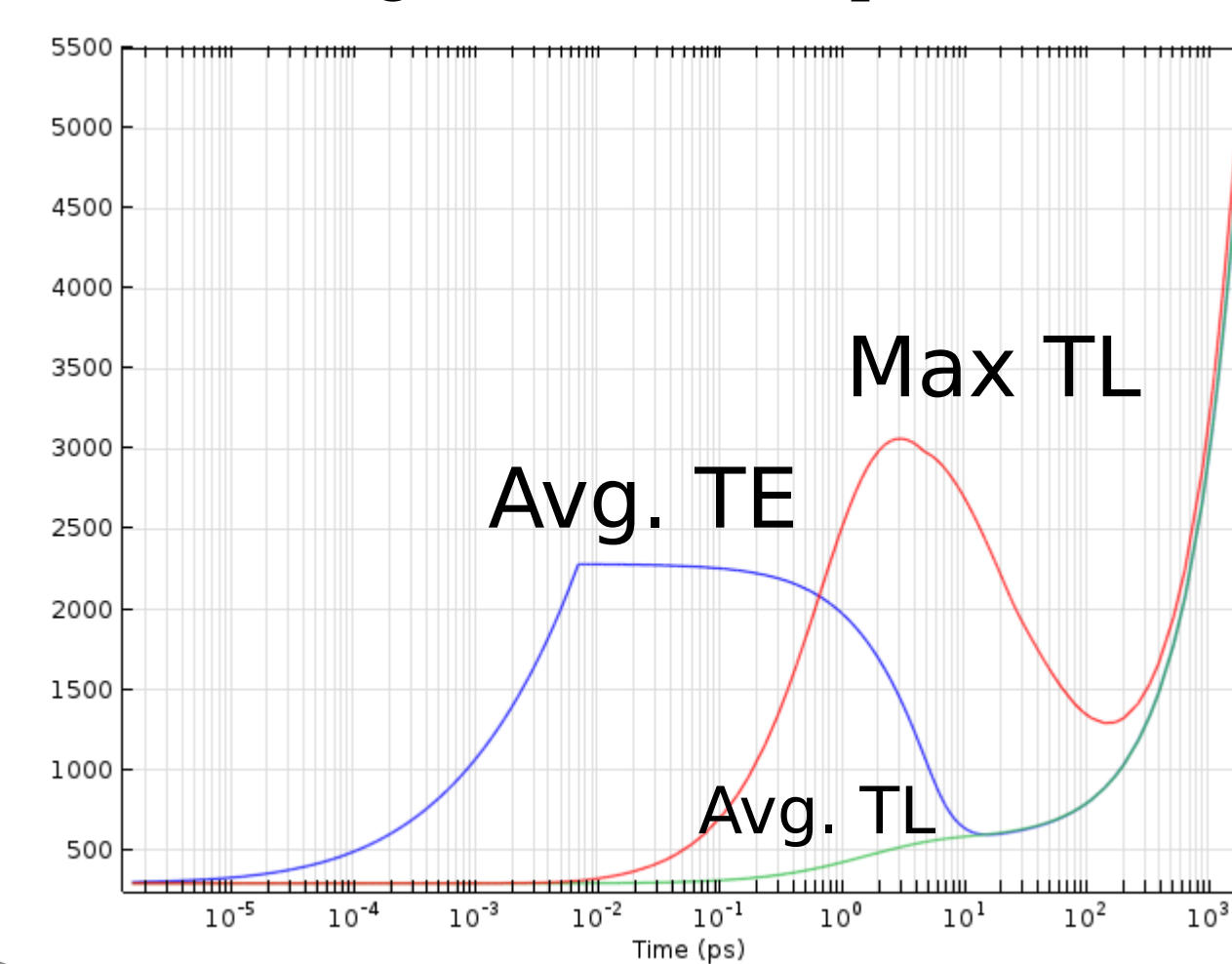
- In high electric fields, emission currents might have a significant effect on the heat distribution.
- We introduce the General Thermal Field equation to the system, along with the Nottingham effect.



Nottingham effect General Thermal Field equation



- Displacement seen on the stress animation increases by an order of magnitude as we cross the melting point of tungsten. At the same point, Nottingham effect flips to cooling mode at the apex



- With the GTF model and Nottingham effect, temperatures start to rise linearly and the tip evaporates. Evidently, a space charge screening must occur, to lower electric fields to some extent and thereby cap the emission current induced heating.

