Molecular Dynamics simulations of nanoscale metal tips under electric fields including electronic processes

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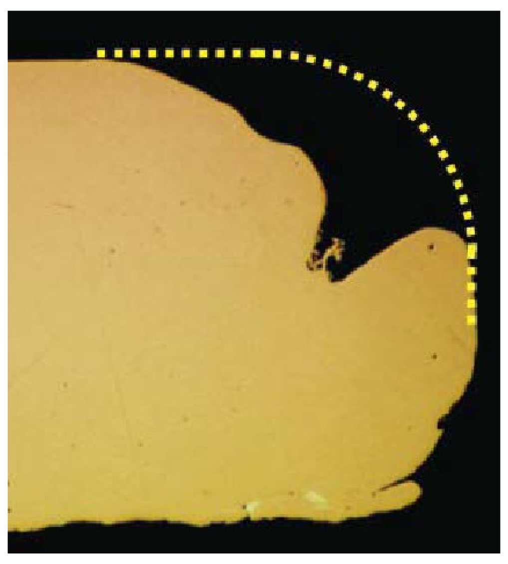
INTRODUCTION

Strong electric fields appear in many modern applications operated at high vacuum, such as particle accelerators and fusion reactors. These strong fields can lead to electric arcs on metal surfaces, which damage equipment and lower their performance.

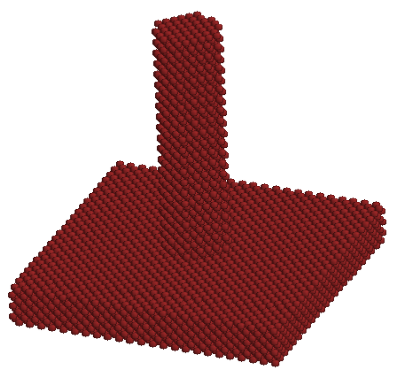


Field electron emission plays a significant role in the arcing phenomenon[1]. Resistive heating, due to the emission current, can cause melting to occur, providing evaporated atoms to build up plasma. If a microscopic protrusion is present on the surface, the threshold of the applied electric field for plasma formation is lower because of the local enhancement of the electric field above the tip.

Classical Molecular Dynamics (MD) simulations do not implicitly include any of the electronic effects needed to simulate the heating that leads to arcing, and therefore these effects must be handled explicitly.

METHODS

A new model for simulating heat processes in a nanotip was implemented into the molecular dynamics code PARCAS. The model includes heating due to field emission currents and cooling due to heat conduction. Thermal radiation is considered negligible.



The temperature the system should have at the next time step is obtained by numerically solving the 1D heat equation

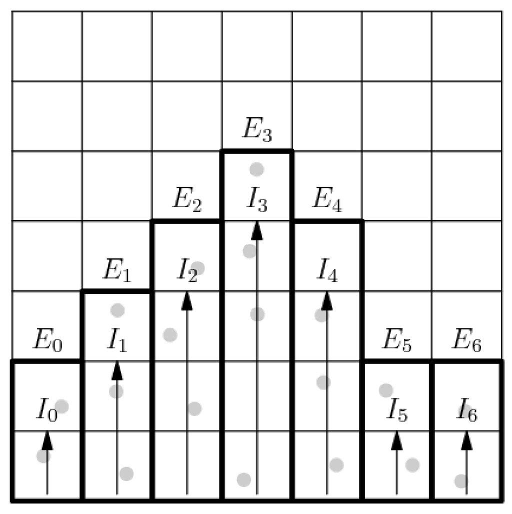
$$\frac{\partial T}{\partial t} = \frac{1}{C_V}\left(\rho(T)J(x)^2 + \kappa_e(T)\frac{\partial^2 T}{\partial x^2}\right)$$

using the finite difference method. This equation describes both the heating and cooling effects on the tip. Once the target temperature is known, the atomic velocities are adjusted correspondingly.

Size-effects strongly affect the electrical resistivity and thermal conductivity. Simulations[2] show that for a tip with a 1nm diameter:

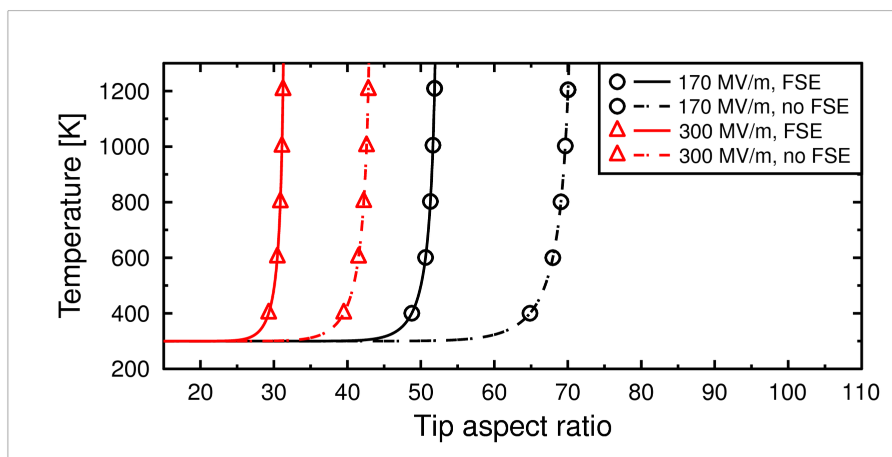
- Resistivity is 65 times the bulk value
- Thermal conductivity is 2% of the bulk value (based on the Wiedemann-Franz law)

In the model, the tip is divided into columns. The electric field above each column is determined and, based on the strength of the field, the total emission current and the current density at each point in the tip is calculated using the Folwer-Nordheim equation



$$J = \lambda_T \frac{aE^2}{\phi\tau(E)^2}\exp\left(-\nu(E)\frac{b\phi^{3/2}}{E}\right)$$

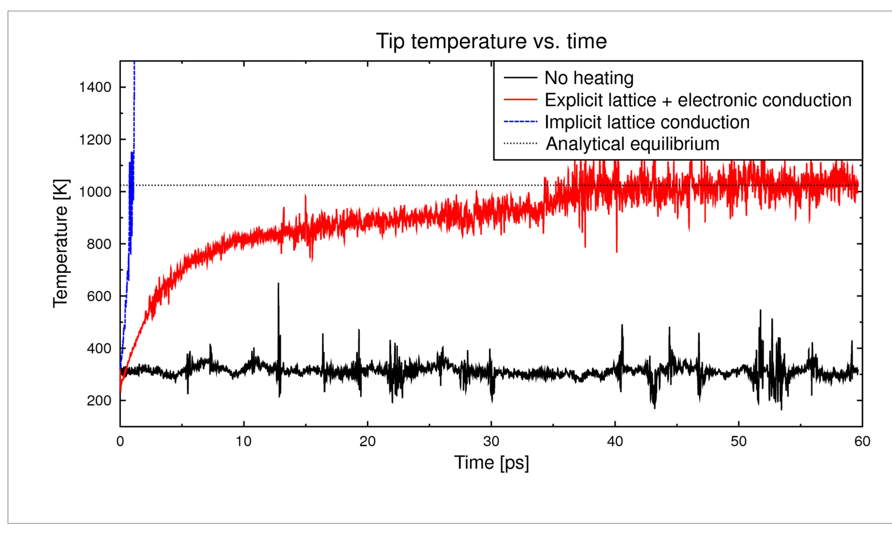
RESULTS



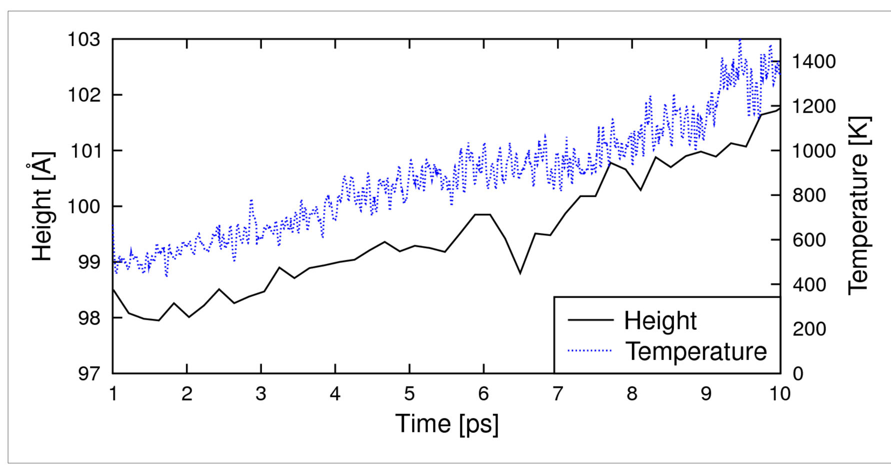
Maximum temperature is a function of tip aspect ratio:

$$T_m = T_B \sec(aJ\beta)$$

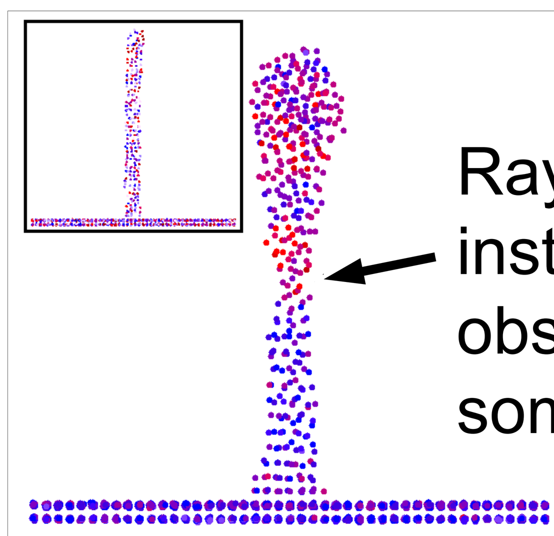
Melting is predicted at experimentally measured breakdown values.



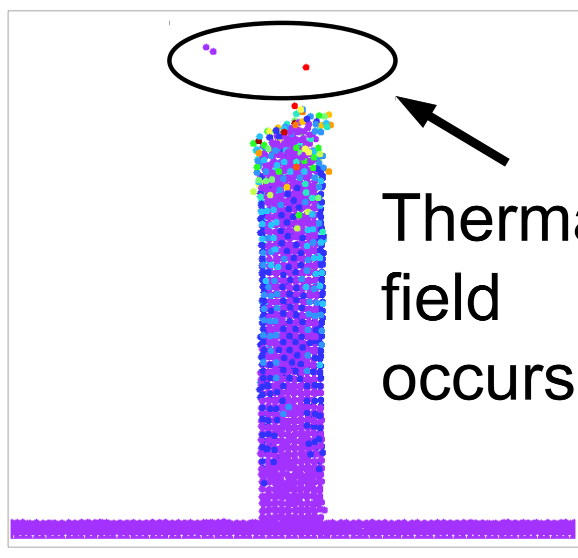
Simulations show that electronic heat conduction must be considered explicitly to obtain analytically predicted temperatures.



A tip is heated and stretched in the presence of an external electric field.



Rayleigh instability is observed in some cases



Thermally assisted field evaporation occurs

CONCLUSIONS

A new model for handling heating in MD was implemented. The model includes heating due to Fowler-Nordheim field emission and cooling due to heat conduction. Simulation results are in good agreement with analytical predictions, which shows that the model works well. Using this model in simulations will provide additional insight into the processes leading to electrical arcing.

References:
[1] D W Williams et al. J. Phys. D:Appl. Phys. (1972)
[2] A. Yarimbiyik et al. Microelectron. Reliab (2009)

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