ELECTRODYNAMICS - MOLECULAR DYNAMICS SIMULATIONS OF THE STABILITY OF CU NANO-PROTRUSIONS UNDER HIGH ELECTRIC FIELD

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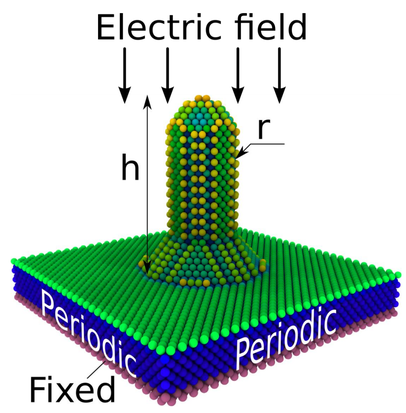
SUMMARY

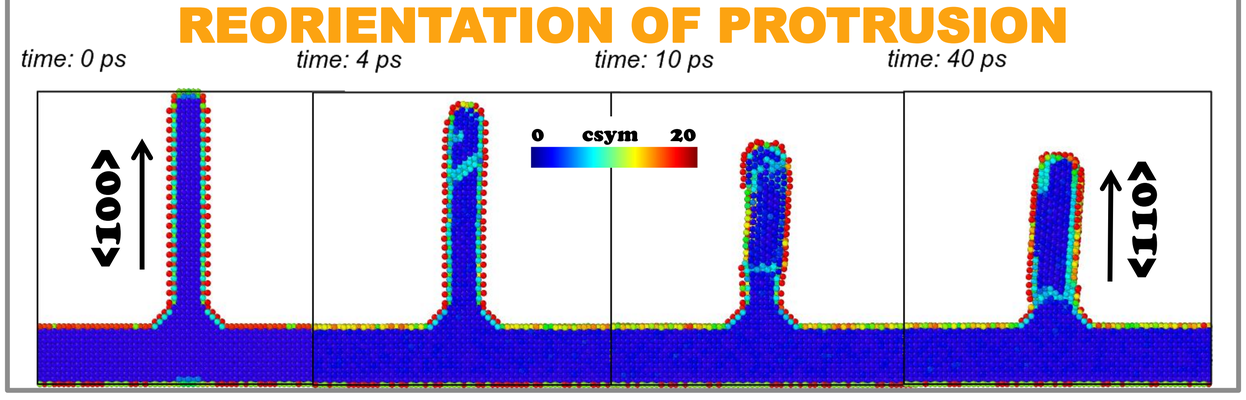
FCC metal nanowires undergo <100>/{001} to <110>/{111} reorientation when exposed to temperature [1] and/or pressure [2] higher than the critical ones. In case of Cu, that transition can be pseudoelastic or exhibit shape memory effect (SME). Although it is well-known that external force acting on a wire can reverse the transition [3], the impact of electric field on the stability of nanowires is unknown. Current study investigates the change of the SME critical temperature in copper on high electric fields. **It is found**, that strong electric field increases the critical temperature significantly, making thus the <100> oriented protrusions **more stable**.

SIMULATION PARAMETERS

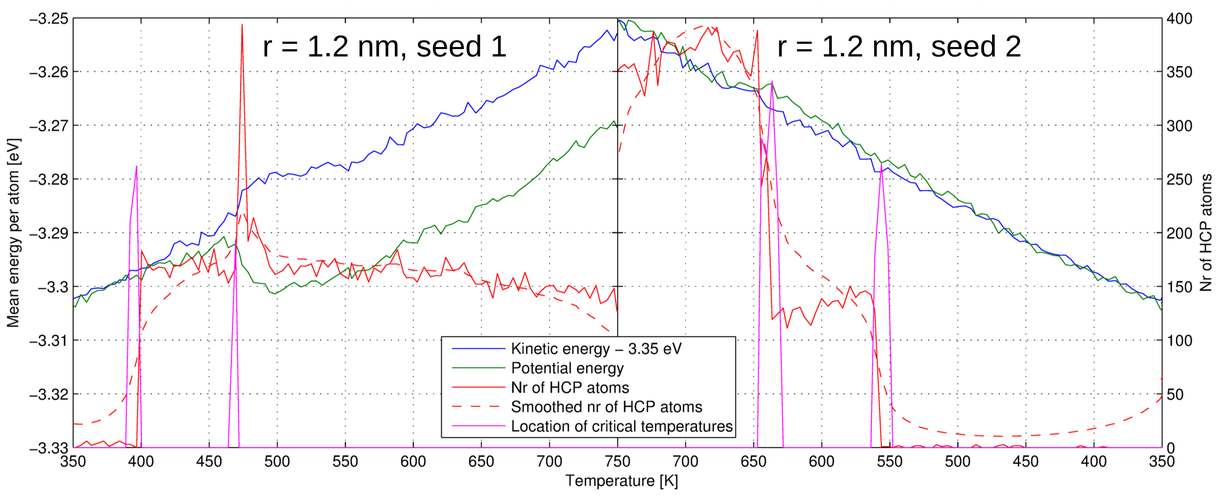
Potential: Mishin *et al* EAM [4]
Temperature ramping rate: 1 K/ps
Initial temperature: ~T_{cr} - 250K
Electric field: 0, 0.5, 1.0, 1.5 GV/m
Radiuses: 1.0-1.4 nm
Height: 6 nm
Relaxation: 10 ps
Simulation time: 410 ps



REORIENTATION OF PROTRUSION

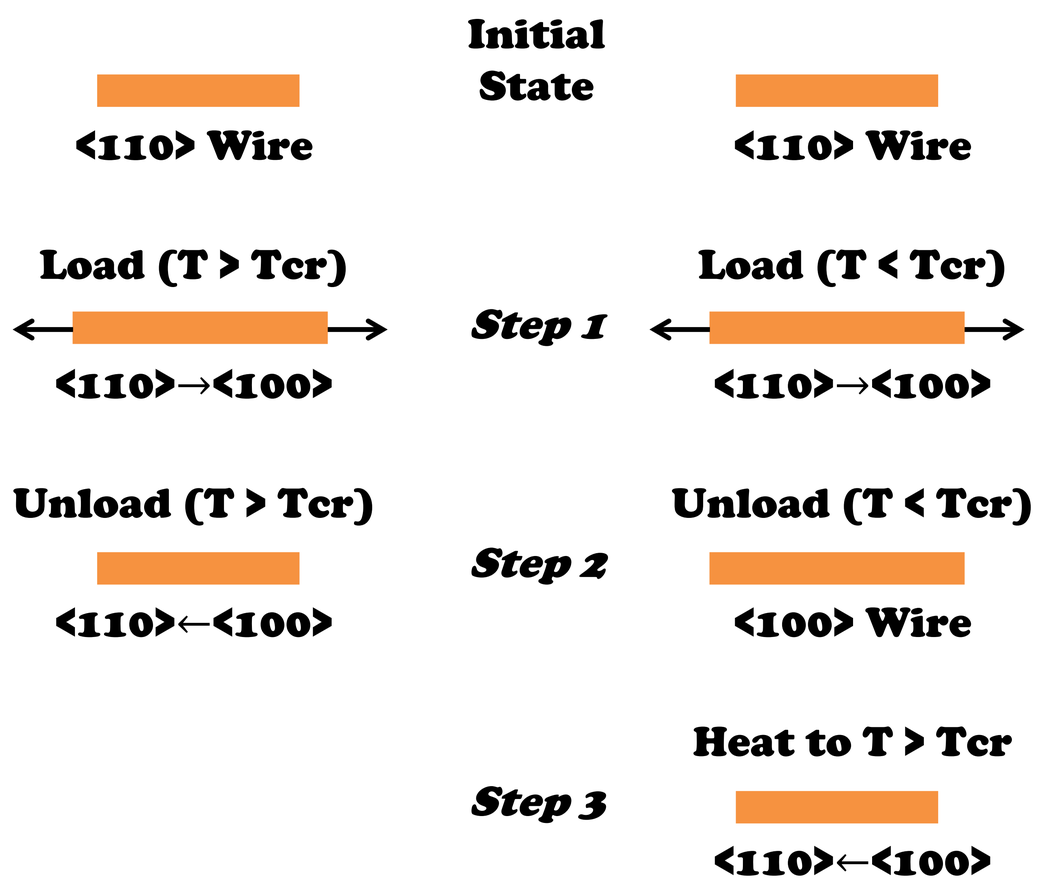


DETERMINING THE CRITICAL TEMPERATURE



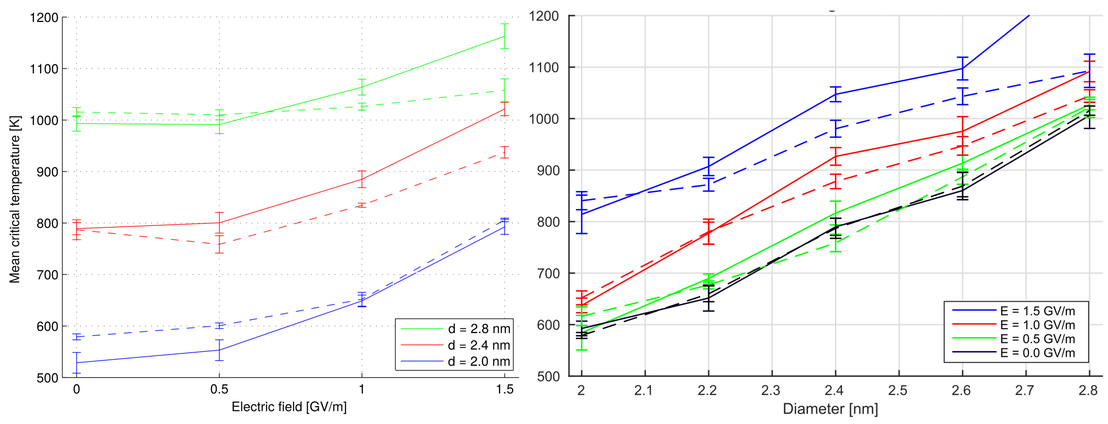
Although the reorientation gets its energy from the energy difference between <100>/{001} and <110>/{111} orientations, the change in mean energy is not always visible. For that reason T_{cr} is determined from the nr of HCP atoms in the system, that is found from common neighbor analysis.

NANOWIRE PSEUDOELASTICITY / NANOWIRE SHAPE MEMORY

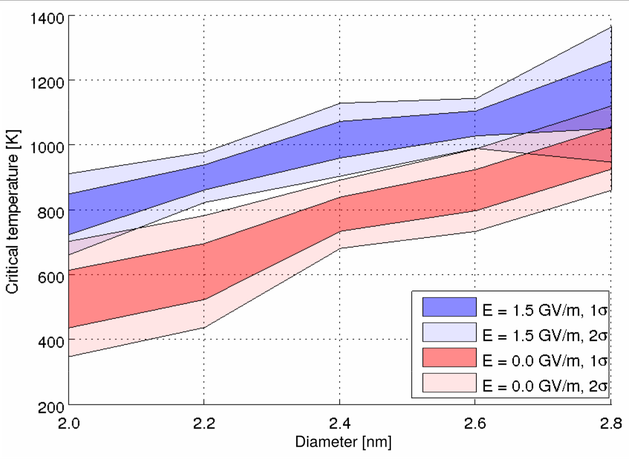


Loading and unloading a copper nanowire transforms its crystallographic orientation reversibly – depending on its temperature it exhibits pseudoelasticity or shape memory. <100> to <110> reorientation is initiated by the surface stress induced by high surface to volue ratio.

CRITICAL TEMPERATURE DEPENDENCE ON ELECTRIC FIELD STRENGTH



Solid line –field currents, electromigration and Joule heating **disabled**
Dashed line – field currents, electromigration and Joule heating **enabled**



1 & 2 standard deviations of T_{cr}

Strong electric field increases significantly SME critical temperature. This gives one possible mechanism, why strong field currents could be measured from Cu surface under high electric field, but no protrusions with high enough aspect ratio are visible with electron microscope.

REFERENCES

[1] W. Liang, M. Zhou, and F. Ke, "Shape Memory Effect in Cu Nanowires," *Nano Lett.*, vol. 5, no. 10, 2005
[2] V. K. Sutrakar, D. Roy Mahapatra, and A. C. R. Pillai, "Temperature–pressure-induced solid–solid ⟨100⟩ to ⟨110⟩ reorientation in FCC metallic nanowire: a molecular dynamic study," *J. Phys. Condens. Matter*, vol. 24, no. 1, 2012
[3] H. Park, K. Gall, and J. Zimmerman, "Shape Memory and Pseudoelasticity in Metal Nanowires," Phys. Rev. Lett., vol. 95, no. 25, 2005
[4] Y. Mishin, M. Mehl, D. Papaconstantopoulos, A. Voter, and J. Kress, Phys. Rev. B, vol. 63, no. 22, 2001.

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