Hydrogen accumulation in copper: hydrostatic effect on dislocations

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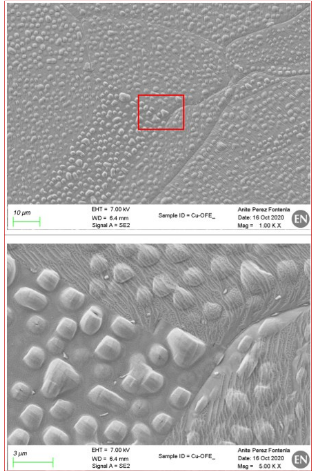
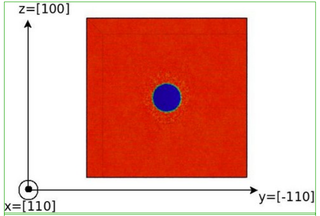
The application of fairly high electric field in accelerating structures leads to surface modification. These areas act as field emitters, and some of them result in breakdowns, carrying the system to the electric disruption. The role of the dislocation activity beneath the surface shows correlation with the breakdown rate [1,2]. The accumulation of H, forming bubbles, acts as new variable to explain the formation of surface protrusion, even at lower fields than the usually applied. The hydrostatic effect of the bubbles enhances dislocation formation, adding up to the tensile stress commonly introduced by the electric field and contributing to the surface modification. Molecular Dynamics (MD) can shed light in this effect, understanding the process of dislocation formation and the eventual surface modification.

Experiments



Experimentally, protrusions appear after low-energy H^- irradiation in Cu

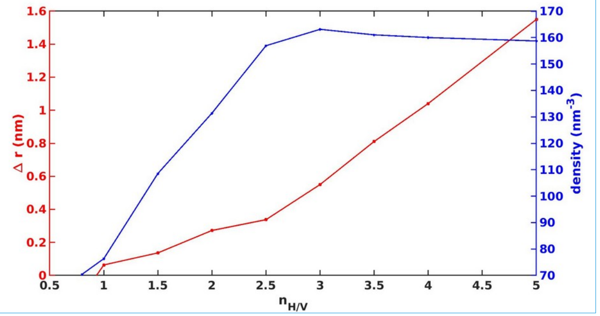
MD model



We introduce different H concentrations, from 0.8 to 5 (H atoms per missing Cu atoms in the void, **n**). We simulate bulk and surface

We can also measure the effect of H when applying a tensile stress (electric field)

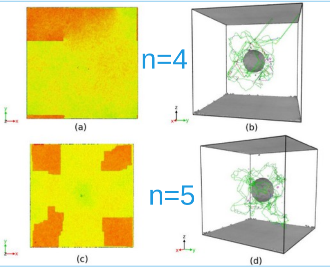
Results - Bulk



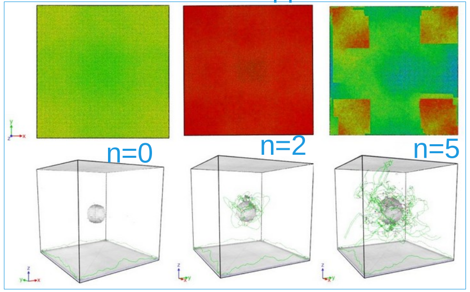
3 different regimes based in the change of the void radius and the H density (n=2.5, 3). Until n=3, the volume grows differently, but not enough to release the pressure.

Results - Surface

We observe that, due to the dislocation created by the pressurize void, the surface yields.



Tensile stress application



We observe that for n=0, no remarkable changes are observed. However it changes when the n>0. The H enhances the creation of dislocation and further surface modification

[1] K. Nordlund and F. Djurabekova, “Defect model for the dependence of breakdown rate on external electric fields,”Phys. Rev. ST Accel. Beams, vol. 15, p. 071002, 2012
[2] E. Z. Engelberg, Y. Ashkenazy, and M. Assaf, “Stochastic model of breakdown nucleation under intense electric fields,”Phys. Rev. Lett., vol. 120, p. 124801, 2018.

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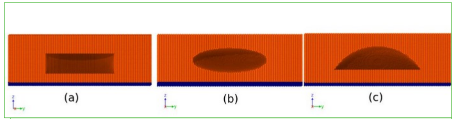
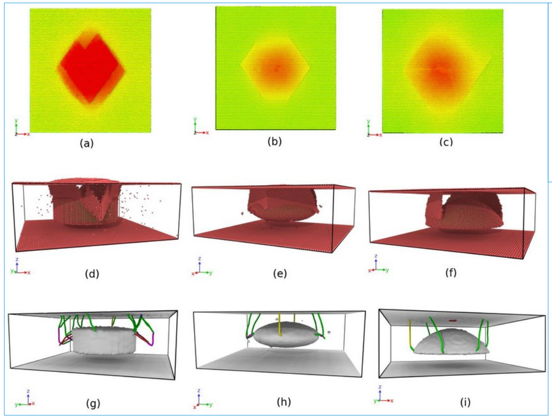
MD model



We introduce n=1.2 H per missing Cu atom. We simulated additionally, two cases using the disk-shape void deeper in the structure for two different concentrations (n=1.2, 2). We can also calculate the atomic stress tensor (virials)

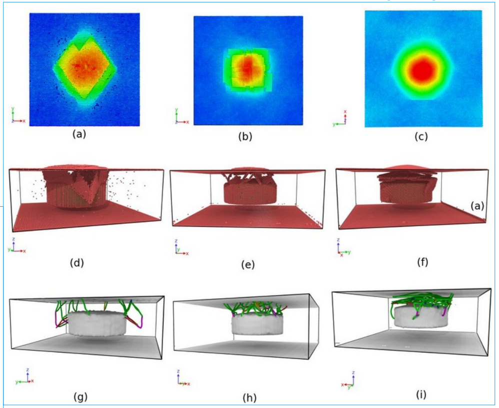
(110)



Results for n=1.2

Protrusion more pronounced in the disk case. The dislocations are created from different places depending on the geometry

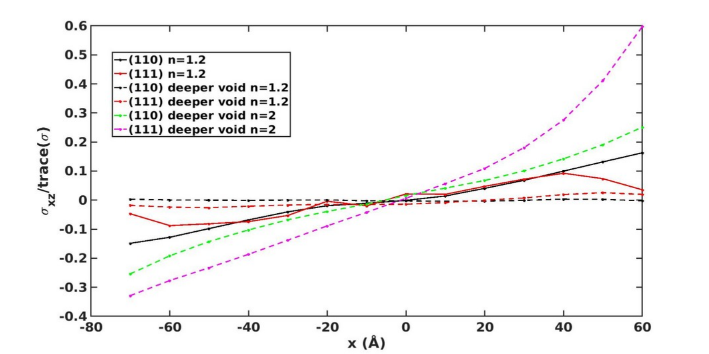
(110) (100) (111)



The protrusion shape is different in each orientation, as it is shown experimentally. The dislocations cut the surfaces differently.

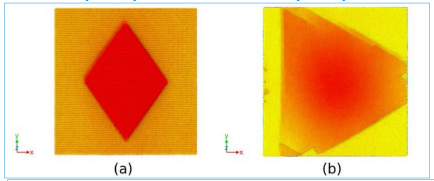
Stress tensor analysis for all the cases

The evolution of the xz component of the stress tensor over the surface of the void in each direction, provides us information on how pronounced, if there is, the protrusion is. The maximum/minimum values of the shear stress coincide with the places were the dislocations are created.



Results for n=2 and deeper void in the cell

(110) (111)



Locating the void deeper in the material requires more H concentration to induce changes in the surface

MD is a suitable tool to understand and follow the dislocation process, specially in this case, dealing with a surface. We have simulated different cases and surfaces orientations. We see the differences between the different orientations. We analyze the response of Cu under hydrostatic or uniaxial tensile stress. We have a powerful tool for study other materials. Other methods, such multi-scale models or DDD, can be used to understand the role of the dislocations in the breakdowns that limit the operation of the accelerating devices.

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