Dislocation interactions in subsurface copper inducing electric breakdowns

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DDD

Discrete Dislocation Dynamics is a mesoscale simulation method where dislocations are interpreted as straight lines connected by nodes which both are inside a uniform solid crystal structure. Each line segment has a determined Burger's vector as well as a stress field. Movement of the dislocations is calculated based on the forces obtained via the Peach–Koehler equation and follows the constraints defined by different crystal system. The approach allows length and time scales up to several micrometers and microsends.

ParaDiS

Parallel **Dis**location **S**imulator is an open source DDD program that has been developed by Lawrence Livermore National Laboratory since 2007. The program has built-in parallelized functions to simulate dislocation movements using the mobility functions for FCC and BCC metals. In the default mode, the simulations are run inside a simulation cell with periodic boundary conditions.

The only crystal defects implemented in the default version are straight dislocations and dislocation loops, along with their interaction with each other. Free surfaces are possible, but they need to be coupled with FEM simulations to be physically realistic.

Our objective is to implement new kinds of defects, such as precipitates, voids and eventually grain boundaries and free surfaces to see how the stacking dislocations cause stress in the near-surface region and eventually induce breakdowns on the surface.

DISLOCATION INTERACTIONS

Hard blocking sphere

The simplest, although non-physical, defect to implement would be a sphere, where the velocity of the dislocation node drops to zero as it reaches the surface of the sphere. This kind of a hard sphere does not correspond to any physical defect, but shows how the free moving parts of the dislocation line are affected by parts which are pinned due to an obstacle.

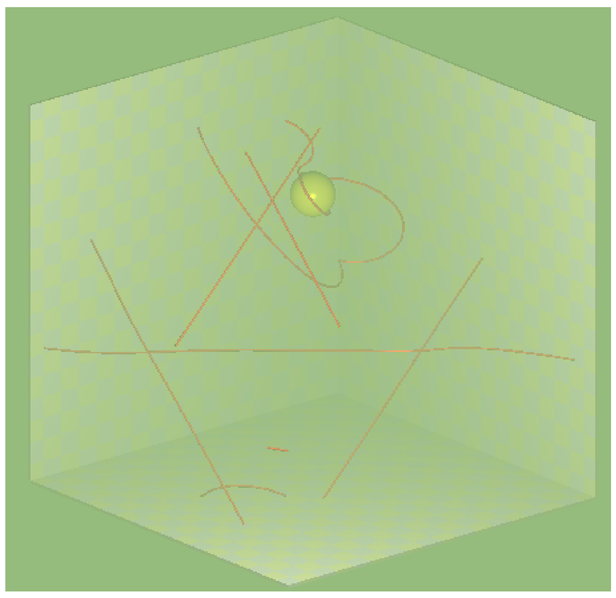

Figure 1: Randomly oriented, moving dislocation lines interacting with each other and colliding with a hard sphere, pinning and changing slip planes.

Precipitates and voids

Another simple, but yet more realistic implementation of a defect would be a Gaussian potential U around a spherical obstacle:

$$U(r) = A \exp\left[-\frac{r^2}{R^2}\right],$$

where r is the distance between the dislocation segment and the obstacle center, R corresponds to the size of the obstacle and A is a strength parameter.

Effect of precipitates and voids inside crystal structure can be approximated by this potential. the The force acting on dislocations is generally repulsive for precipitates and attractive for voids.

The type of the collision varies with the paraameters A and R. If A is small, the dislocations pass trhough the obstacle without much of an effect, but with large A, they are forced to stop on the surface or change a slip plane.

Stacking Fault Tetrahedra

SFTs are commonly observed in treated FCC metals and they also act as obstacles for moving edge and screw dislocations. The interaction depends strongly on the geometry and the crystal temperature. A passing dislocation may damage the SFT, possibly leading to dissolution of the obstacle.

Grain boundaries

On a grain boundary, the crystal orientation changes, which makes the collisions with dislocations a complex phenomenom. The possible modes of the interaction include dislocation absorption, reflection and transmission as well as combinations of all three. The calculation requires understanding of at least the Burger's vectors, glide planes and stress fields on both sides of the interface.

Free surfaces

When the dislocations are located in a finite medium, additional forces are applied on them on the surface. These forces can be calculated from image stresses, which again can be estimated by coupling the DDD simulation with FEM simulations.

DC PULSE EXPERIMENTS

A DC pulsing system almost identical the Large Electrode System in CERN has been recently installed in Helsinki. The first measurement are able to start shortly, with the aim in confirming the obsercvations from the simulations.

Sample types

Currently there are three types of electrodes to be tested.

- **Soft Cu**
  The electrodes are annealed close to their melting point in order to create large crystals and grains.
- **Hard Cu**
  Hard copper refers to commercial copper, which is only machined to the correct shape. The crystal structure is more amorphous and the grain size much smaller compared to soft copper.
- **He implanted Cu**
  Copper samples implanted with He atoms in order to generate voids in the bulk.

Conditioning algorithm

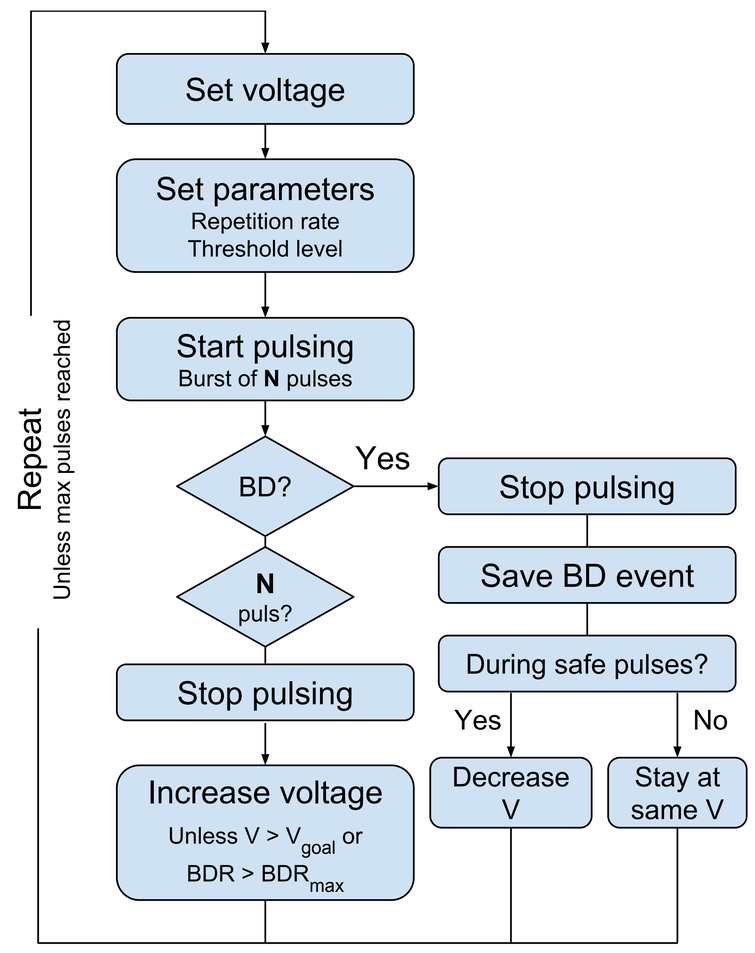

Figure 2: The conditioning algorithm

The algorithm is designed to run as long as the breakdown rate at the goal voltage is larger than a desired level. Characteristics of the material can be obtained from graphs showing the electric field and voltage as function of the number of pulses generated.

DC experiments in CERN show that hard Cu conditions much faster compared to soft.

FUTURE WORK

In addition to confirming the results from the LES experiments in CERN, the system in Helsinki will be used to condition electrodes treated with different methods. For example annealing only a surface layer or a half of the electrodes.

Also the ParaDIS code is developed to be able to simulate effect of the various obstacles on moving dislocations.