Aarne Pohjonen*
Flyura Djurabekova
Kai Nordlund
Antti Kuronen

Helsinki Institute of Physics (HIP) and
Department of Physics
P.O.Box 43 FIN-00014
University of Helsinki, Finland

*e-mail:aarne.pohjonen@helsinki.fi

Steven Fitzgerald

Culham Centre for Fusion Energy,
Abingdon
OX123DB, Great Britain

Dislocations emitted from void under tensile stress – growth on surface

INTRODUCTION

The accelerating electric field strength in linear colliders is limited by occurrence of electric breakdowns. This limit depends on surface electric field. [1] Experiments have shown that the electric field applied to metal surface is enhanced locally at random spots [2]. This local field enhancement can be explained by the formation of sharp features on the surface. Such sharp features cause the initiation of the plasma arc as described in fig. 2 [3]. In the current work we focus on the first stage of the process and try to understand the initiation of the breakdown.

Earlier studies show that a void inside metal grows under shock loading due to dislocation loop emission from the void (fig. 1) [4]. In studies of microparticles in an electrically stressed vacuum gap, marks probably caused by a gas bubble bursting just beneath the surface after a current flow have been observed (fig. 3) [5]. Numerous holes have also been seen on an aluminium anode where particles seemed to have originated (fig. 4) [6].

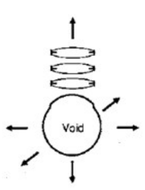

Figure 1. [4]

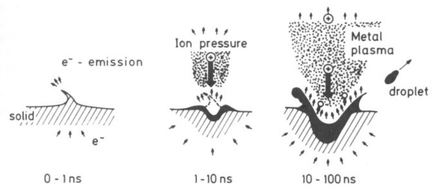

Figure 2. [3]

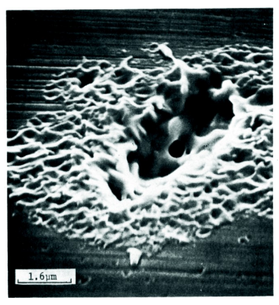

Figure 3. [5]

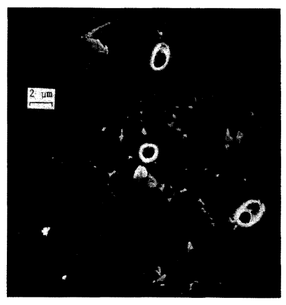

Figure 4. [6]

Hypothesis: if a void is located near surface, the dislocation emission may lead to mass shift of the volume located above the void.

Our MD simulations show that such mass shift indeed can happen. When pulling force is exerted on surface atoms we have observed and identified dislocations emitted from the void. Critical depth dependence on the void radius has been found.

METHODS

We have performed molecular dynamics (MD) simulations to investigate the possibility of growth on the surface due to dislocation nucleation from a void in copper below (110) surface under stress:

A void was placed in the simulation cell below surface at 600 K temperature. Stress was applied on the two top layers of atoms corresponding to a pressures of 4.58 GPa. Simulation time was 420 ps. Stacking faults were identified by using centrosymmetry analysis [7]. The stress was ramped linearly during 100 ps after 20 ps relaxation of the system.

A set of simulations were made for determining the so-called critical depth dependence on the void radius with different stresses. The critical depth is defined as the largest depth of the void where mass shift is observed. Also the temperature dependence of the critical depth was systematically investigated under 4.58 Gpa stress and the elastic energy density of the system was investigated by applying the stress in 0K and plotting potential energies of the atoms.

RESULTS

We observed stacking faults related to the dislocation nucleation on the void by the centrosymmetry analysis. The dislocations caused shift of the volume above the void (figure 5). The tip shape (viewed from above) shows the orientation of the dislocation lines (figure 6)

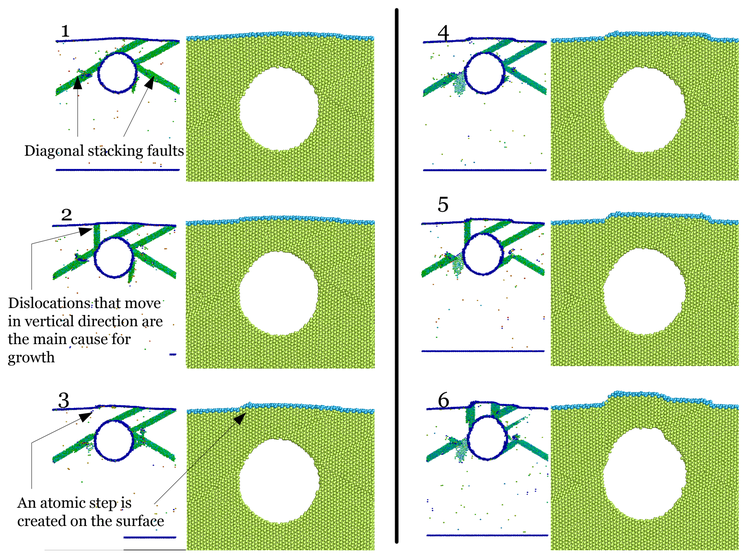

Figure 5.

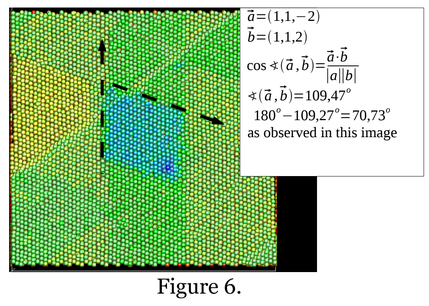

Figure 6.

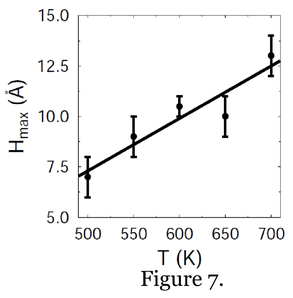

Figure 7.

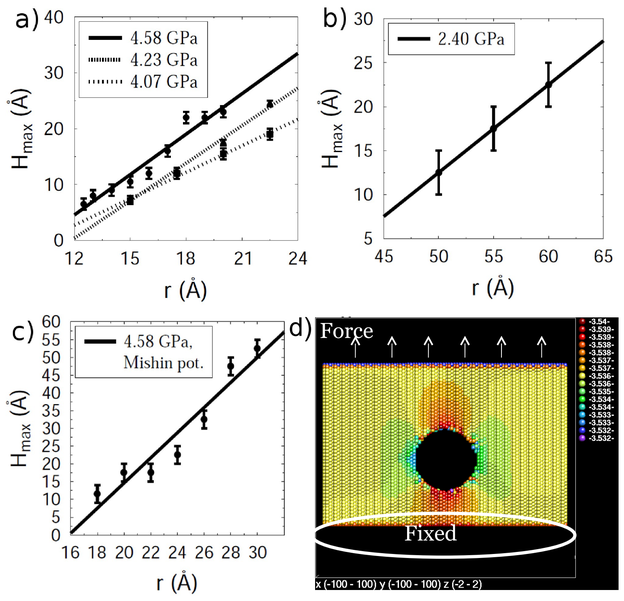

Figure 8.

The atoms in figure 8 are colored by the potential energy of the atom, showing the elastic energy density of the system [8]

$$U=\frac{1}{2}\sum_{\lambda=1}^{6}\sum_{\mu=1}^{6}\tilde{C}_{\lambda\mu}e_{\lambda}e_{\mu}$$

where e_λ and e_μ are the strain components and $\tilde{C}_{\lambda\mu}$ are related to the elastic stiffness components by $C_{\alpha\beta}=\frac{1}{2}(\tilde{C}_{\alpha\beta}+\tilde{C}_{\beta\alpha})=C_{\beta\alpha}$

We have investigated the critical depth dependence on temperature (figure 7) and on radius of the void applying different stresses (figure 8 a,b,c) with MD simulations. The following criterion for growth was observed:

Criterion for growth

Growth will occur during timescale Δt if

$$h < a(r - r_{\min})$$

where

h is the depth of the void

r is the radius of the void

$r_{\min}$ is the minimum radius for the growth to occur

CONCLUSIONS

A void located below (110) surface under stress was found to emit dislocations with <112> line directions under stress which cause growth of a tip on the surface. The dislocations glide on {111} planes as expected [9] for FCC crystals. We have found that the growth of the tip depends on the depth and radius of the void as stated by the criterion for growth. The linear dependence can be understood by the fraction of area above the void to the area that connect the cylindrical volume to the bulk. The critical depth was found to depend approximately linearly on temperature under 4.58 Gpa stress in the simulated time scale.

Any questions?
I would be happy to answer them!
Send me mail:
aarne.pohjonen@helsinki.fi

References:

[1]: Wuensch, W. *Observations about RF Breakdown from the CLIC High-Gradient Testing Program*, CLIC Note 700
[2]: Boxman, R. L., Martin, P.J., Sanders D. M. *Handbook of vacuum arc science and technology*
[3]: Behrisch, R., *Surface erosion by electrical arcs,* Max-Planck institut für plasmaphysik, EURATOM association.
[4]: Ahn, D. C., Sofronis, P., : *Void growth by dislocation-loop emission*. Journal of Applied Physics, 101, 063514 (2007)
[5]: Theophilus, G., van Heeswijk, R., and Srivastava, K., IEEE Transactions on Power Apparatus and Systems PAS-94, 1859 (1975).
[6]: Menon, M. and Srivastava, K., J. Appl. Phys. 45, 2094 (1974).
[7]: Knap, J. and Ortiz, M., Phys. Rev. Lett. 90, 226102 (2003).
[8]: Kittel, C., *Introduction to Solid State Physics*, John Wiley & Sons, Inc, New York, 3rd edition
[9]: Hull, D., Bacon, D. J., *Introduction to Dislocations*, Butterworth Heinemann, Oxford, 4th edtion

HELSINGIN YLIOPISTO
HELSINGFORS UNIVERSITET
MATEMAATTIS-LUONNONTIETEELLINEN TIEDEKUNTA
MATEMATISK-NATURVETENSKAPLIGA FAKULTETEN