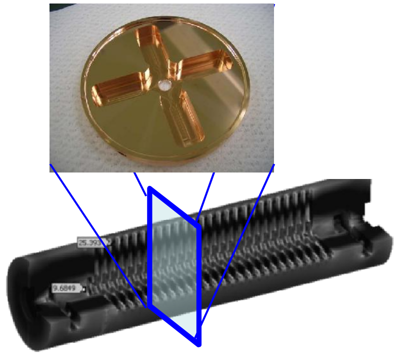
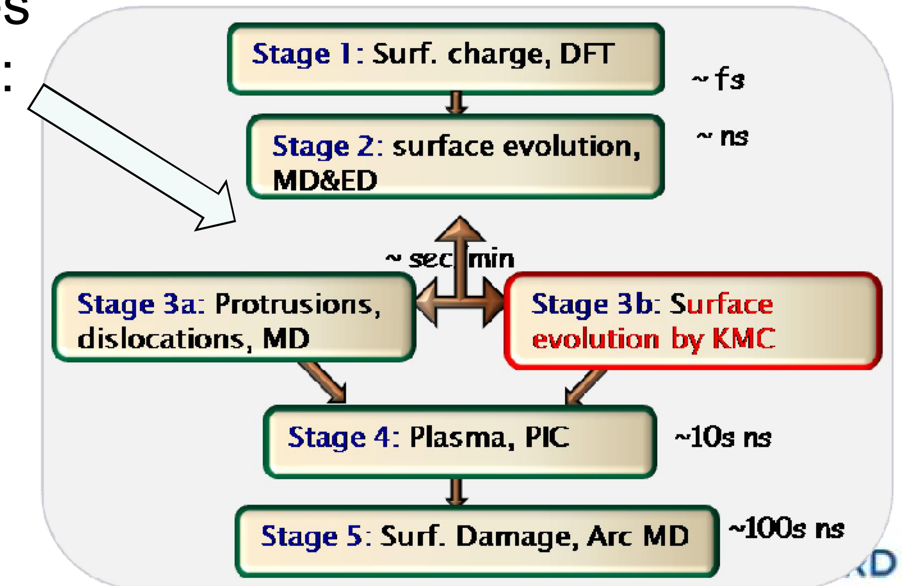
WP9.2 Sub-task 3: Multiscale modeling of break-down in CLIC RF structures

HELSINGIN YLIOPISTO
HELSINGFORS UNIVERSITET
UNIVERSITY OF HELSINKI

F. Djurabekova (HIP/UH), V.Zadin (Univ. of Tartu, Estonia), A. Pohjonen (HIP/UH), S. Parviainen (UH/HIP), A. Ruzibaev (HIP), K. Nordlund (UH/HIP); in close collaboration with W. Wuensch (CERN)



- CLIC RF structures: one of major challenges electrical breakdowns near structure surface under very high electric fields.
  - developing a **multiscale model** to understand the mechanisms in or close to the surface of the materials due to the effect of static electric field.
- Currently pursuing parallel activities in all steps of the *multiscale* model:
  - simulating plastic deformations of metal surfaces due to tensile stresses leading to tips on the surface
  - combining electrodynamic effects atomistic simulations to predict behavior of surface atoms;
  - simulation of created plasma and subsequent surface damage.



Current focus: material model from atomistic to macroscopic properties

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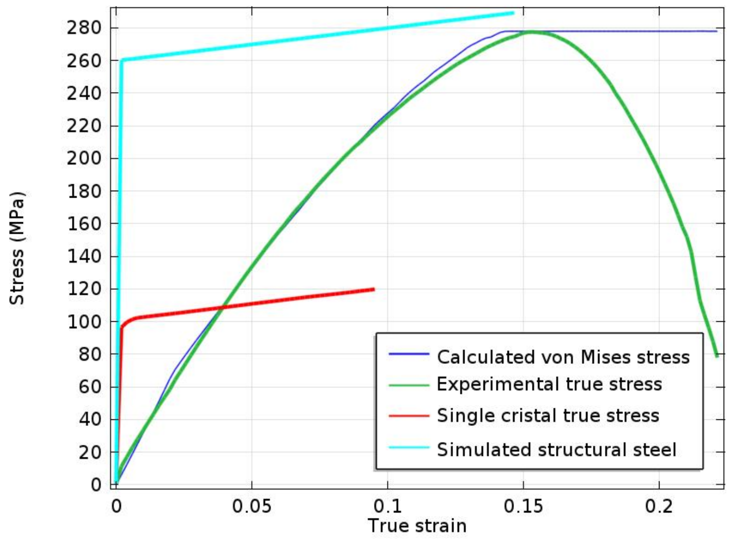
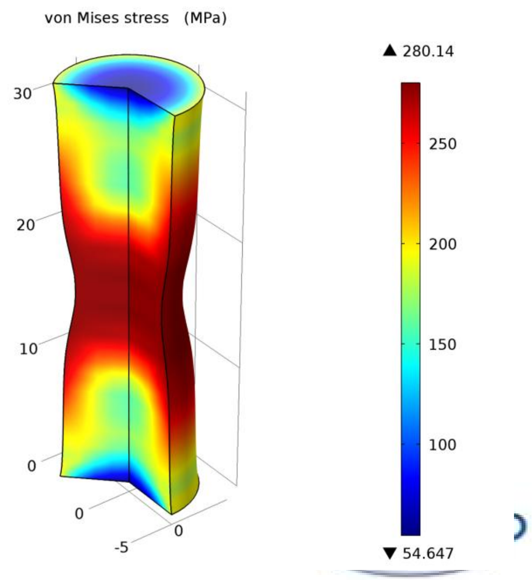
- Using **COMSOL** software for **FEM** calculations estimate relevance of proposed void-based mechanism for a protrusion growth by modeling macroscopic Cu mechanical properties.
- Results:
  - Elastoplastic deformation of material, simulation of large strains
  - Validation of material model and parameters by conducting tensile stress simulations
  - Accurate duplication of the experimental results

Parameters from tensile test macroscopic, single crystal parameters needed due to large grain size



	Structural Steel	Soft Copper (CERN)	Single crystal copper	Often used copper parameters
Young modulus	200 GPa	3.05 GPa	57 GPa	110 GPa
Initial yield stress	260 MPa	68 MPa	98 MPa	70 MPa

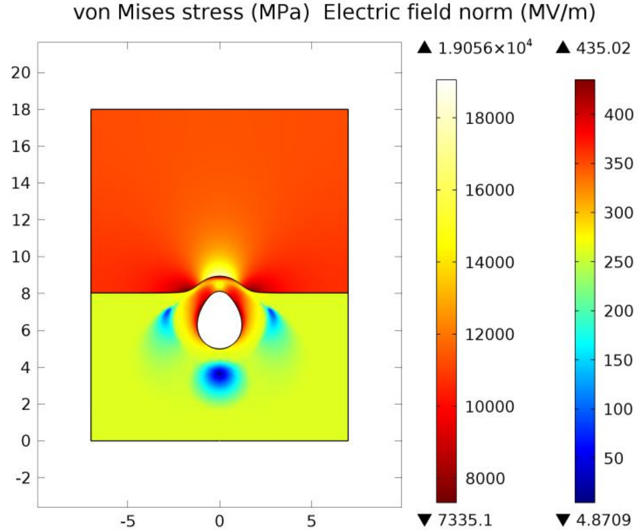


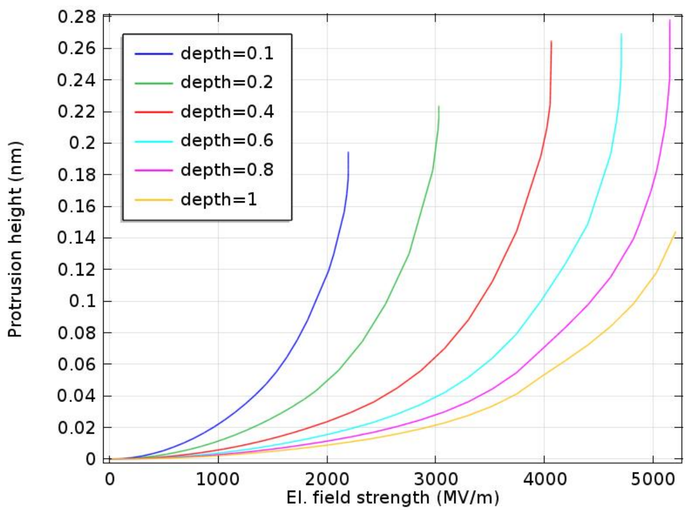
CLIC

Plastic deformation & protrusion formation

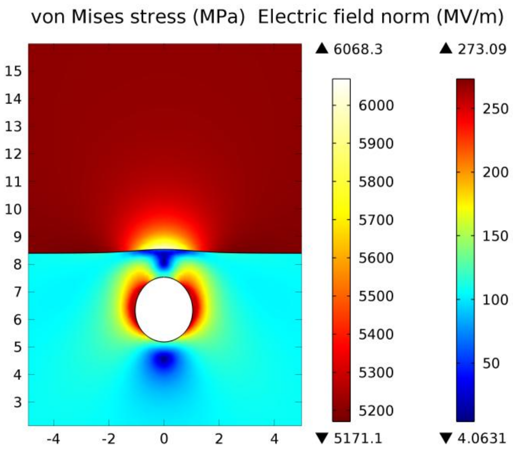
- Scale invariance – larger voids produce only larger protrusions
- Well defined protrusion evolves on the steel surface
- Low protrusion evolves on the soft copper surface
- Protrusion formation on copper surface requires ~2 times lower electric field
- Soft material "harder" to deform
  - Material hardening around void
  - Nearby material deformed due to low Young modulus
- Over 2 MV/m required to initiate any significant protrusion formation in soft copper

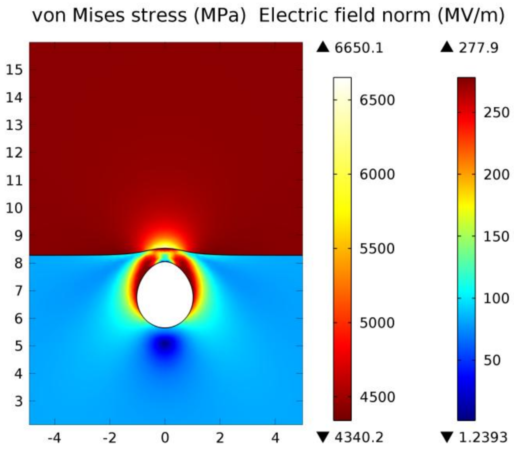
Structural steel





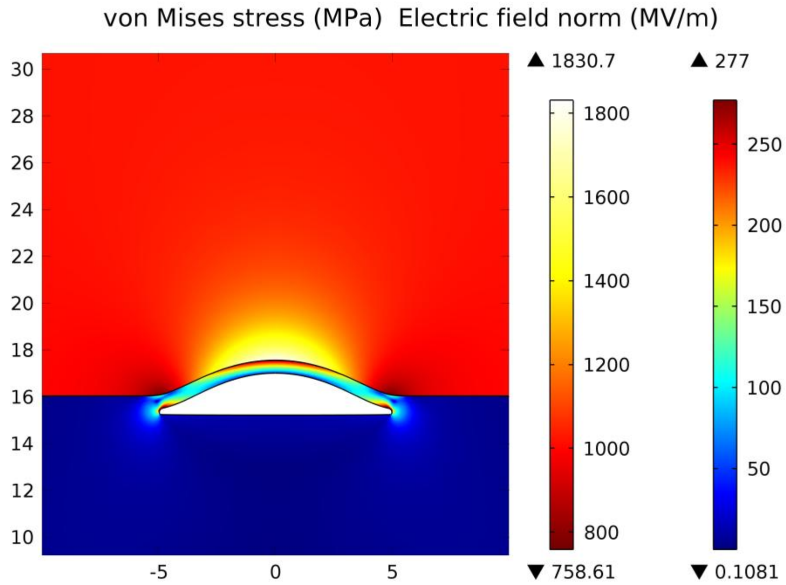
Soft copper

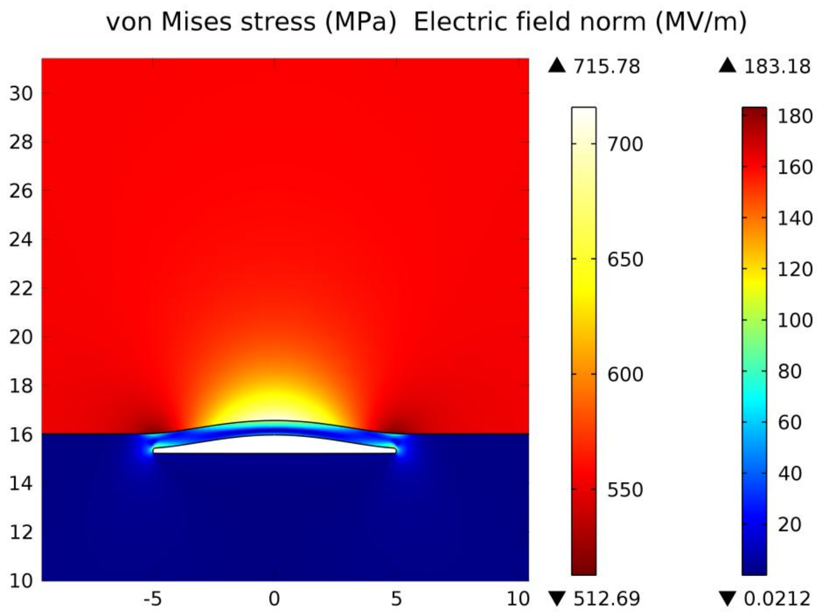




Deformation at realistic electric strength

- Protrusion formation starts at fields > 400 MV/m
- Material plastic only in vicinity of defect
- Thin slit may be formed by combination of voids or by a layer of fragile impurities

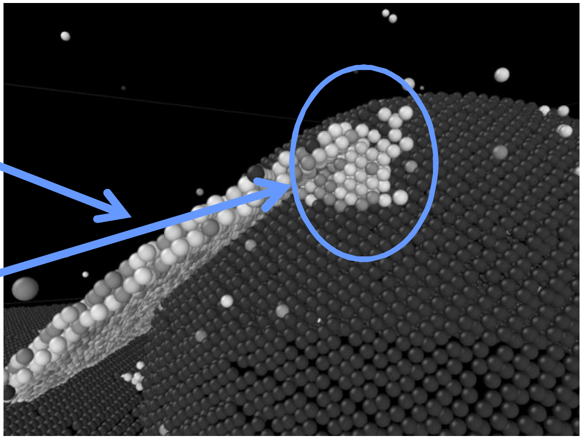




- Field enhancement factor ~2.4
- Thin material layer over the void acts like a lever, decreasing the pressure needed for protrusion formation

Calculation of activation energy for nucleation of dislocation

- A set of simulations on hemispherical voids in single crystal structure with the {110} surface has been set to estimate the activation volume and activation energy for the nucleation of dislocations. The process of nucleation of a dislocation has a complex nature.
- The slip planes in off-perpendicular direction release the partial dislocations, forming stacking faults. These stacking faults always precede nucleation of the dislocation in the perpendicular direction to the surface.



- Now collecting bigger statistics of such events with the purpose to calculate the actual stress at the point of nucleation as well as the required activation volume.
- The results will help for time estimation of the process

Future activities

- **Dislocation activities:**
  - Finalize the calculation of activation energy of nucleation of a dislocation on a stress concentrator -> publication
  - Study of dynamics of dislocations at the near-surface void will be summarized in a PhD thesis to be defended in 2013
  - Systematic assessment of the elastic-plastic response of the macroscopic materials on the external electric field with the aid of FEM (COMSOL) calculations.
- **Comparison of Electron densities from quantum & classical model:** Submit the publication on *work function* results, obtained by first principles techniques (Density Functional Theory, DFT) for different surfaces with/without self-adatoms on surface. This result will be compared to the experimental measurements of the work function by the laser irradiation of Cu surfaces.
- **Electric field effects**: Submit the manuscript on the comparison of results obtained by hybrid ED-MD code and Atom Probe tomography experiments.

WP9.2 sub-task 5: precise assembly

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L. Kortelainen & K. Österberg, HIP; in collaboration with G. Riddone & F. Rossi (CERN)

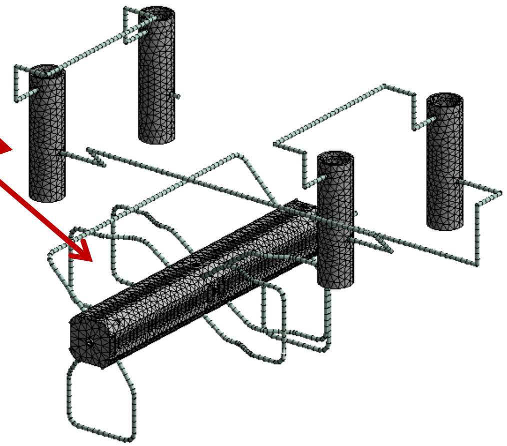
Thermo-mechanical modelling of CLIC two-beam module

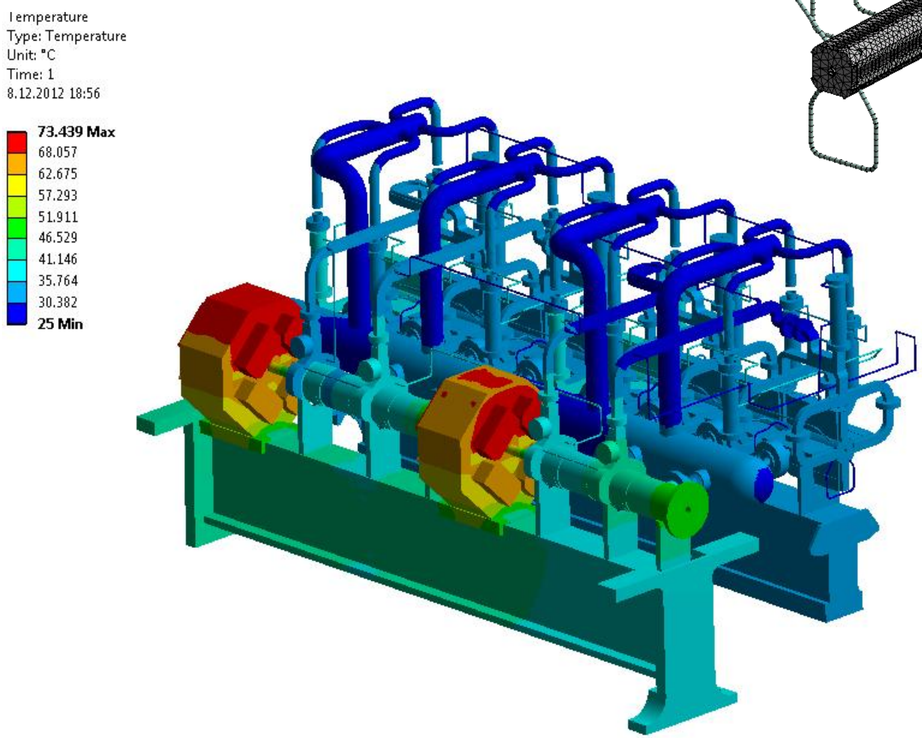
✓ Improving thermo-mechanical model of CLIC lab test module #0 (TM0)

- cooling channels for compact loads & power dissipation to DBQ added

- parametrisation of mass flows, water inlet temperatures & heat dissipations $\rightarrow$ prediction of temperature during different operation conditions:

accelerating structures and compact loads with cooling channels





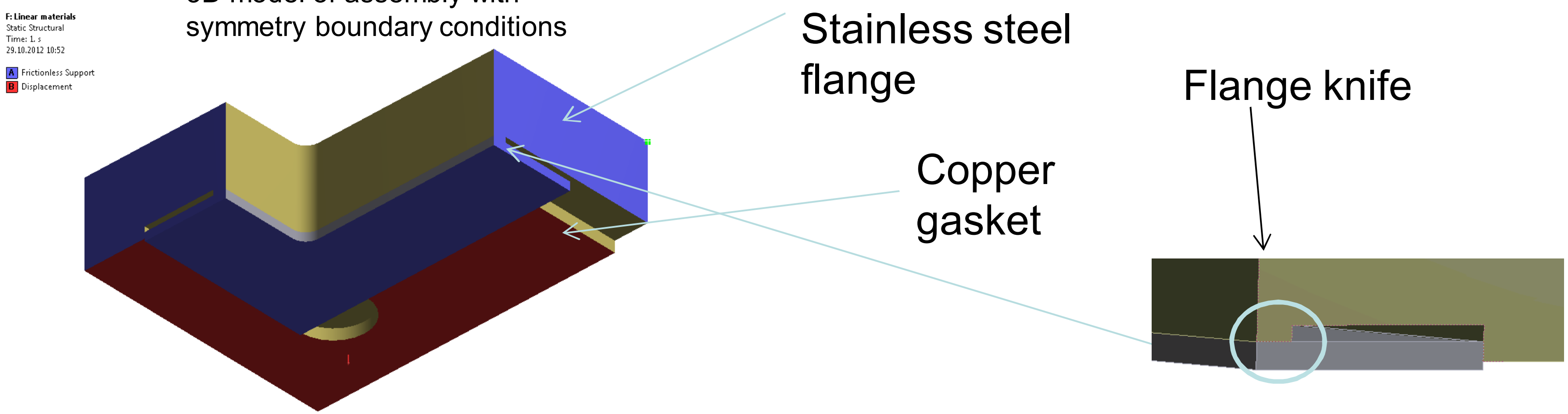
temperature distribution in lab test module #0 during baseline operation

EuCARD

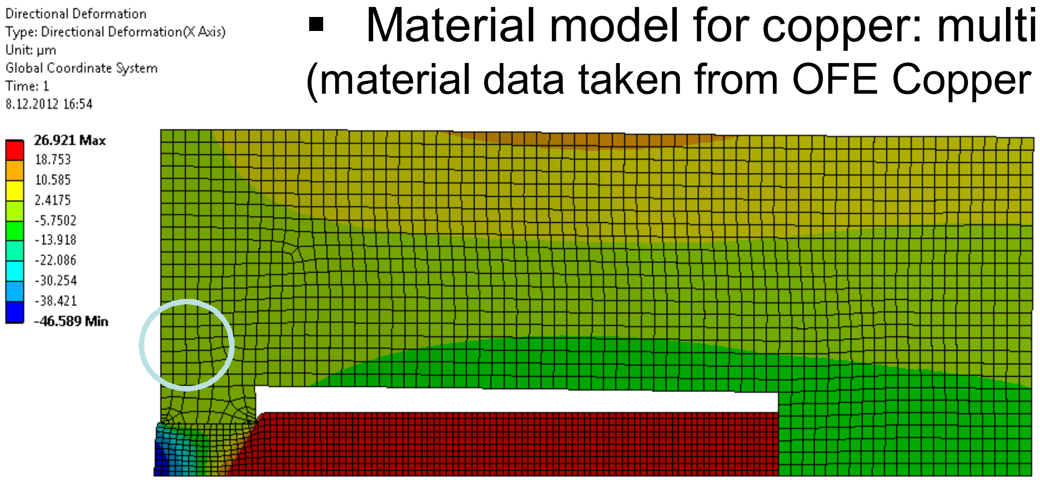
IUWR90 flange simulation

- Assembly contains two flanges & one copper gasket which is compressed between the flanges to prevent leakages

3D model of assembly with symmetry boundary conditions



- Plane stress case with symmetry boundary conditions was simulated with different flange knife dimensions according to the 2D drawing received
    - Material model for copper: multilinear isotropic hardening (material data taken from OFE Copper uniaxial tests, EDMS: 1241837)



Next steps

Lab test module # 0

- Define more input/output parameters to the model
- FEA model of bellows (to check stiffness values provided by manufacturer)

IUWR90 Flange

- 3D simulation of the assembly