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Molecular dynamics simulations of surface damage in CLIC?

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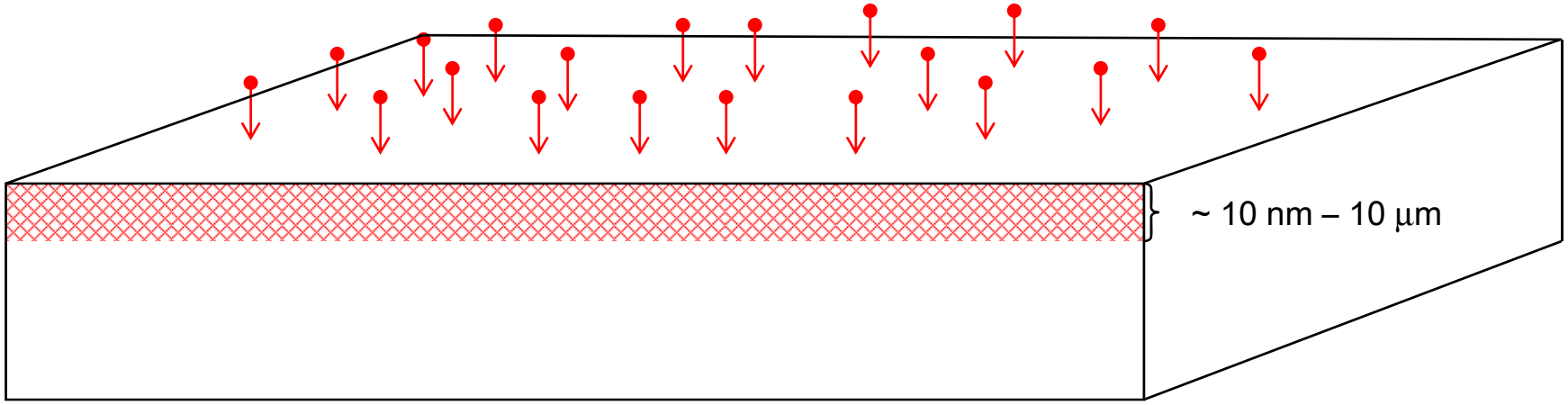
- MD simulations: features and feasibility
- Agreement of the previous MD predictions to experimental results
- Relevance to CLIC component damage?
- Plans and an algorithm for the model of spontaneous roughening
- Timetable

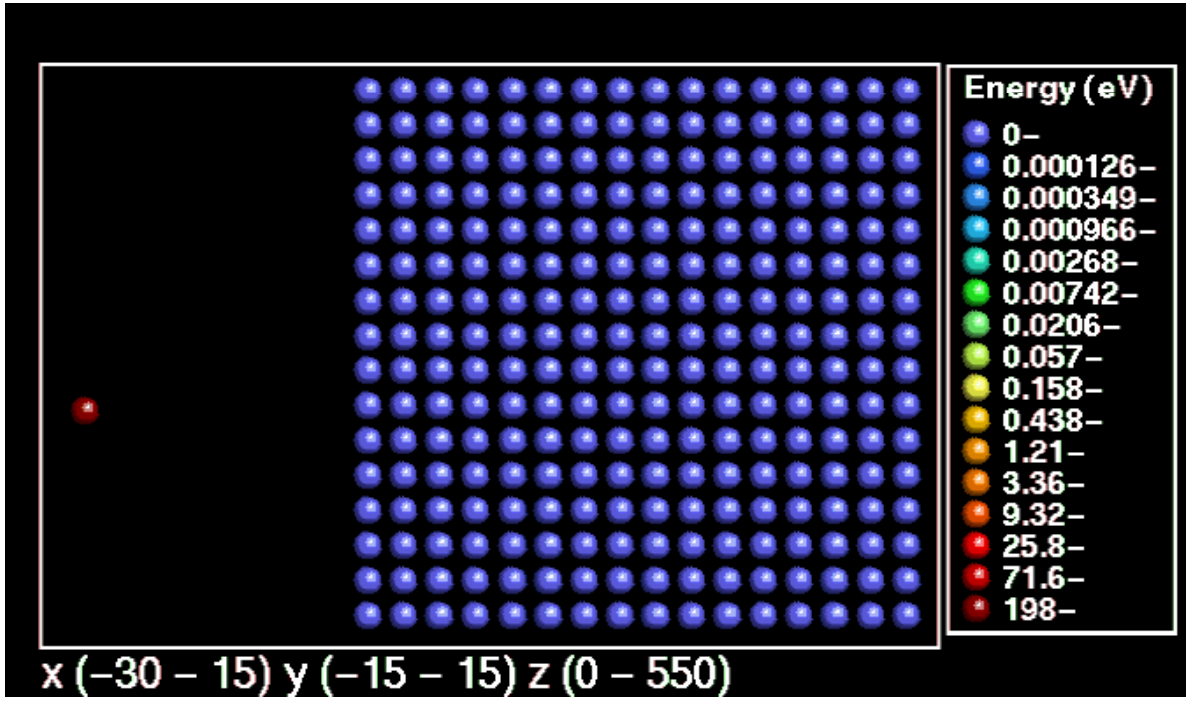
Ion and cluster irradiation of materials

- We come from accelerator laboratories focusing on materials physics
- Basic question: what happens when an ion or cluster ion accelerated to an energy of 10 eV – 50 MeV enters a material:
  - Damage on surface? Damage in bulk?
  - Beneficial effects: doping of semiconductors, optical effects…



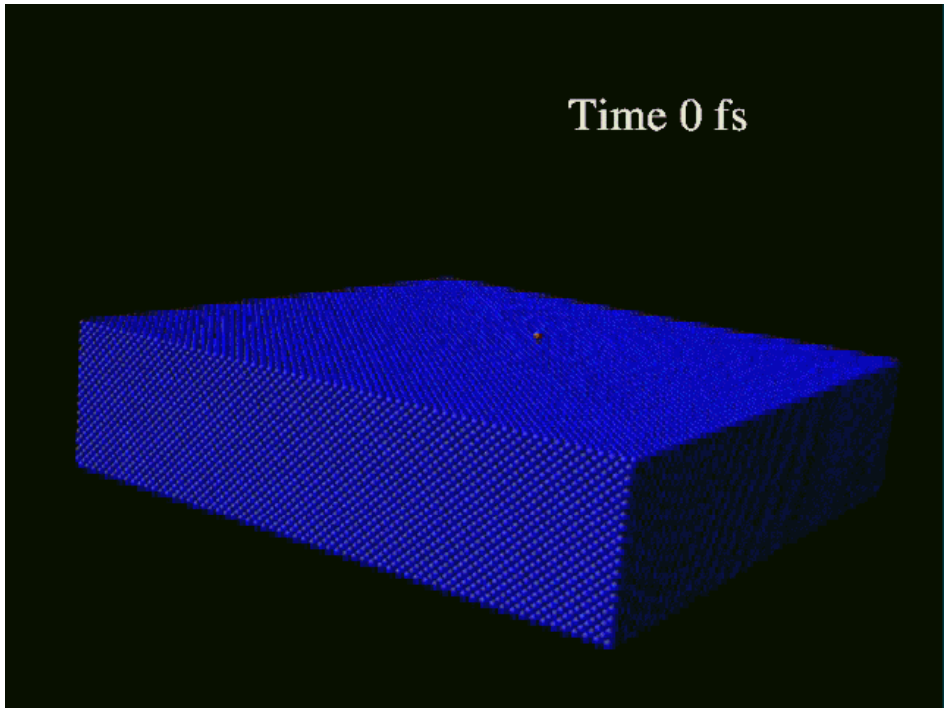
Atomistic simulations of irradiation effects

- Atomistic simulations can give insight into what really happens when energetic particles interact with surfaces
- Example: atom motion when 500 eV Au hits Cu



Bigger energies: massive surface damage

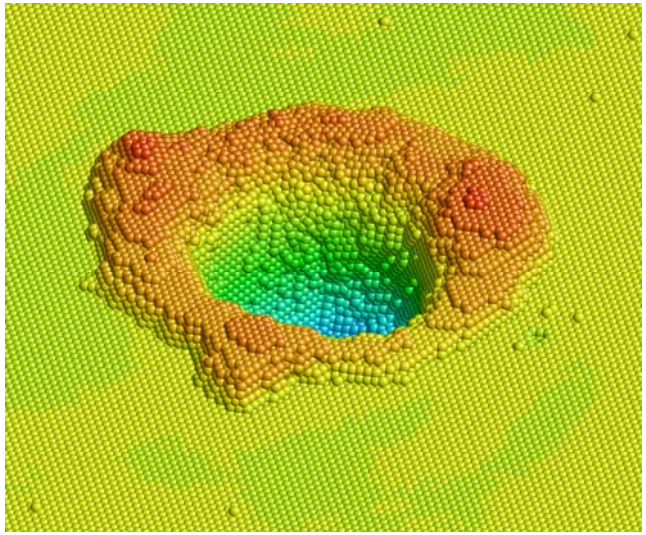
- For heavy ion bombardment and dense metals, a single incoming ion may lead to really dramatic surface effects



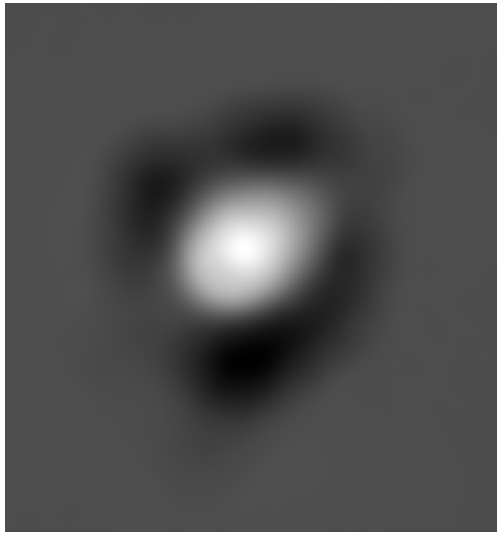
Surface damage: cratering

- The typical end result is a crater
- The craters we get in simulations can be directly compared to experiments by predicting the transmission electron microscopy (TEM) image of it

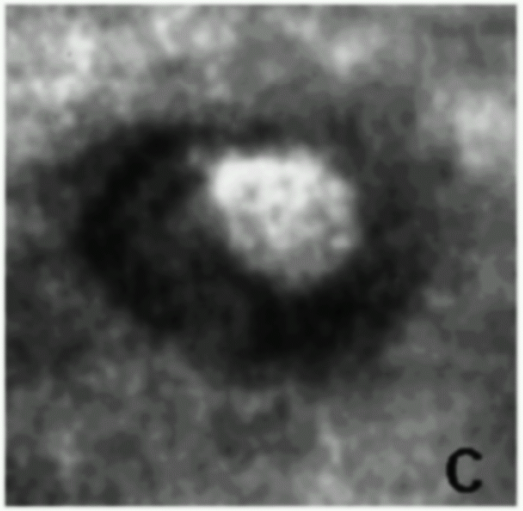
MD simulation result



Predicted TEM image



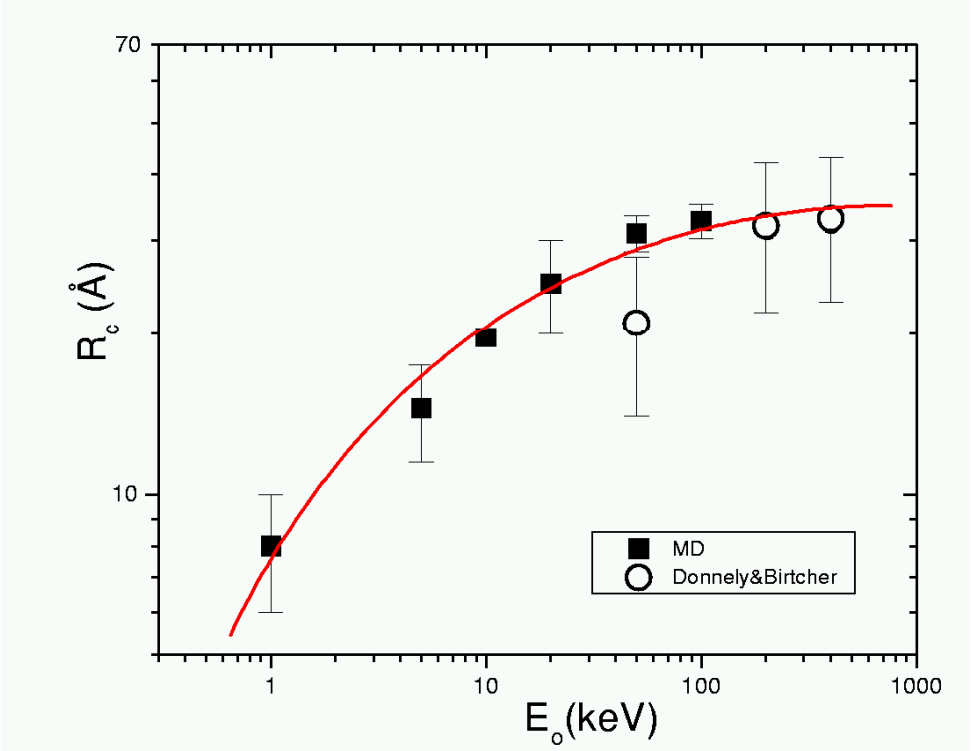
Experimental TEM image



[Donnelly, Physical Review B **85** (1997) 4968]

Surface damage: cratering

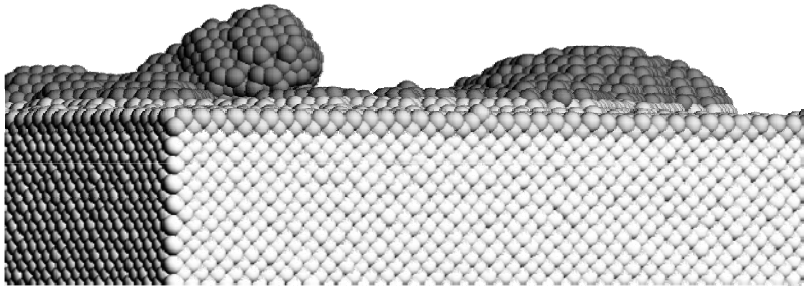
- A quantitative comparison shows the crater sizes we get agree well with the experimental ones

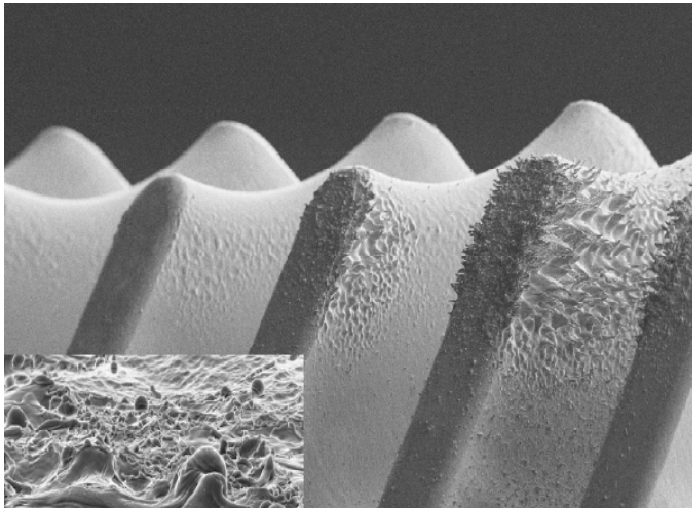


[Bringa et al, Phys. Rev. B 64 (2001) 235426]

Relevance to CLIC component damage?

- Any stray heavy particles in the CLIC accelerating cavities could *in principle* be ionized at the surface, accelerated in the plasma or over the electric field, and cause surface damage like that shown in the animations
  - Some of the surface damage we get, resembles that in CLIC components
  - But the scale is nm rather than microns

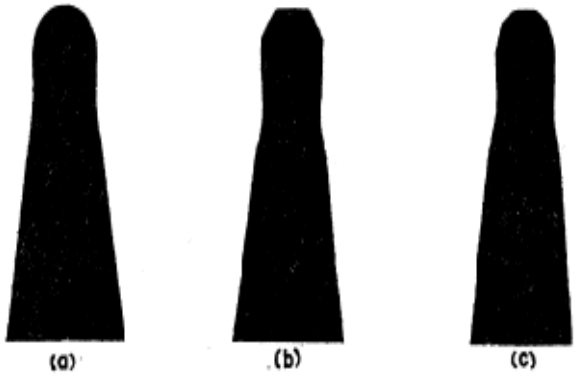




[Walter Wünsch, CERN]

Plans for simulating CLIC damage: spontaneous roughening?

- To study the onset of rf breakdown in CLIC, we consider is electric-field induced spontaneous surface roughening
- It is known that at least at high temperatures, metal tips can spontaneously sharpen when a high electric field is applied on them [Bettler, Phys. Rev. 119 (1960) 85]



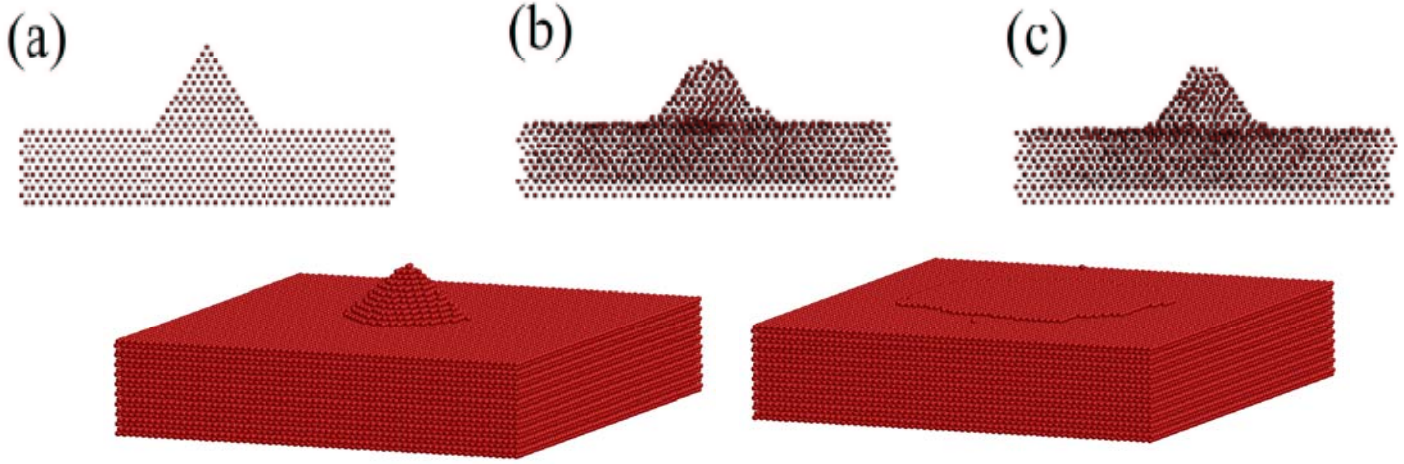
  - Could this also occur at low temperatures in the CLIC conditions? Could explain the onset of roughening?

Hybrid atomistic – electrodynamic simulation model

- We plan to simulate the issue using an approach similar to that developed at Argonne Natl. Lab. [Z. Insepov] to simulate cluster emission from a tip
- Sketch of planned algorithm:
  1. Simulate one ordinary molecular dynamics time step => gives equilibrium forces between atoms $\boldsymbol{F}_{equi}$
  2. Obtain radius of curvature of every atom
  3. Obtain total charge in simulation cell from external electric field $\boldsymbol{E}(t)$ and hence charges on surface atoms q_i
  4. Calculate electrostatic forces between charges $\boldsymbol{F}_{q}$
  5. Get image forces from charges to metal surface $\boldsymbol{F}_{if}$
  6. Add up total force $\boldsymbol{F}_{tot} = \boldsymbol{F}_{equi} + \boldsymbol{F}_{q} + \boldsymbol{F}_{if}$

Spontaneous tip smoothening?

- On the other hand, when no electric field is applied, we know that nanosize Cu tips dullen and flatten out spontaneously due to surface diffusion [Frantz, J. Phys. Cond. Matter 16 (2004) 2995]
  - Could this explain why they have not been seen?
  - We can extrapolate our results of small clusters to bigger ones to estimate what size features would vanish



Timetable

- The implementation of the hybrid MD-electrodynamic model will begin in Jan 2008
  - Challenging:
    - Electrostatics terms not part of usual MD
    - Stability of MD algorithms under external forces not well known, special temperature control algorithms may be needed
    - ED equations for image charges gives a divergence at z=0 that must be controlled
- Aim to be able to run test simulations in spring 2008, production runs in mid and late 2008.