[Computer simulation of] possible materials modification effects by very high-flux accelerated ions

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Presentation of our groups

Prof. Kai Nordlund
Principal investigator

Doc. Antti Kuronen
Principal investigator

Doc. Flyura Djurabekova
Principal investigator

Working with CERN, ITER / EUROFusion, FAIR, ORNL, …

Research results since 1998:

- **~ 550 publications**
- **37 PhD theses**

Dr Andrea Sand
Fusion reactor mat'ls

Dr Andrey Ilinov
Ion beam processing

Dr Fredric Granberg

Dr Ville Jansson

Dr Andreas Kyritsakis

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Nanoclusters

M Sc Ekaterina Baibuz
Particle physics mat'ls

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FeCr interfaces

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Fusion reactor mat'ls

M Sc Alvaro Lopez
Surface ripples

M Sc Mihkel Veske
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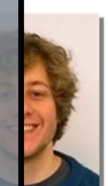
Particle physics mat'ls

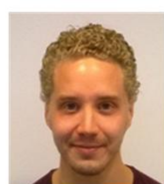


M Sc Henrique Vazquez
Swift heavy ions

M Sc Christoffer Fridlund
Ion beam processing

M.Sc Jesper Byggmästar
Fusion reactor mat'ls

M.Sc Jian Liu
Graphene and DLC



M.Sc Emil Levo
Fusion reactor mat'ls

M.Sc Jyri Lahtinen
Machine learning

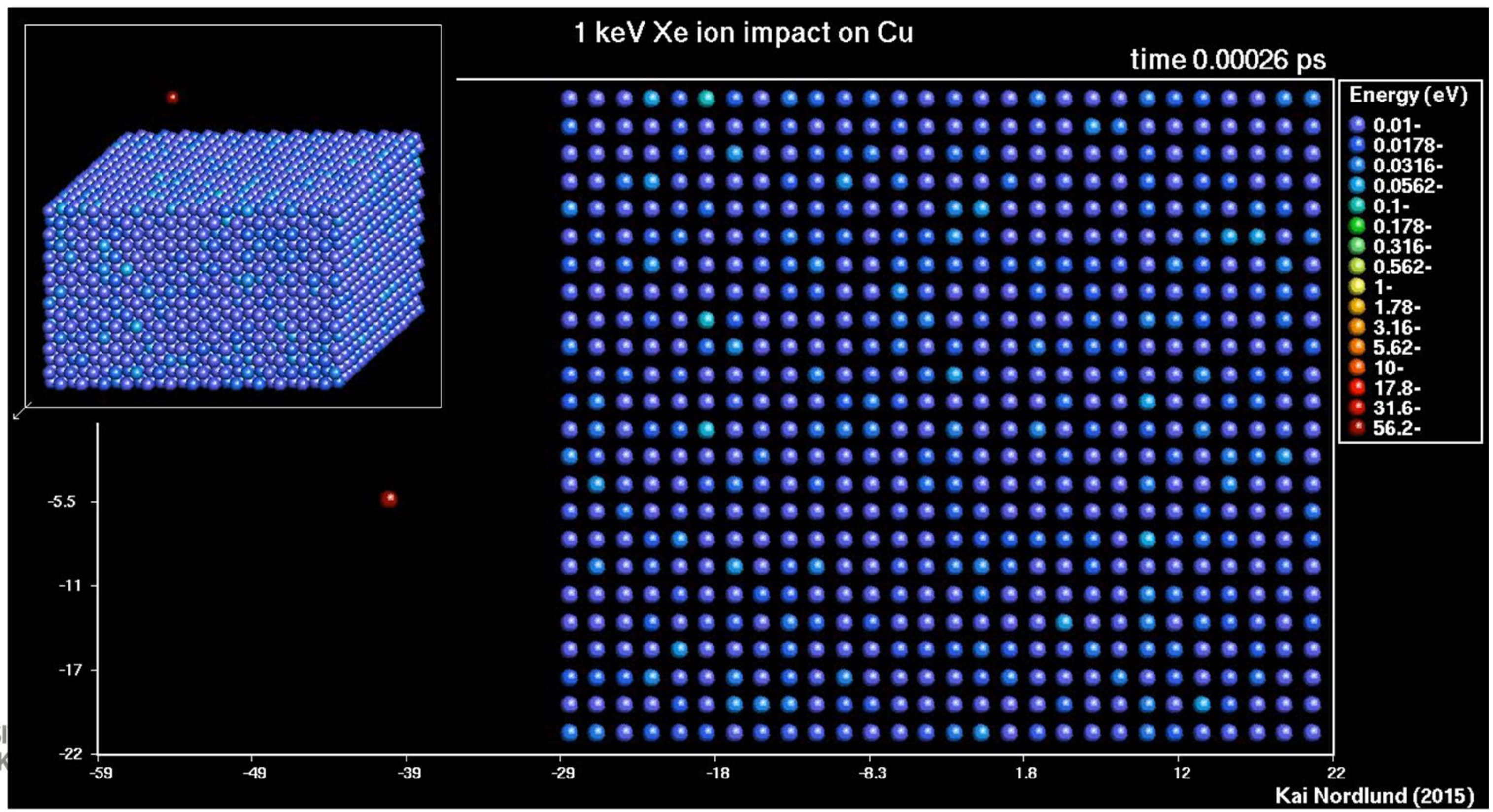
M.Sc. Anton Saressalo
Arcing experiments

B.Sc. Ville Jantunen
Swift heavy ions

B.Sc. Jonna Romppainen
Particle physics mat'ls

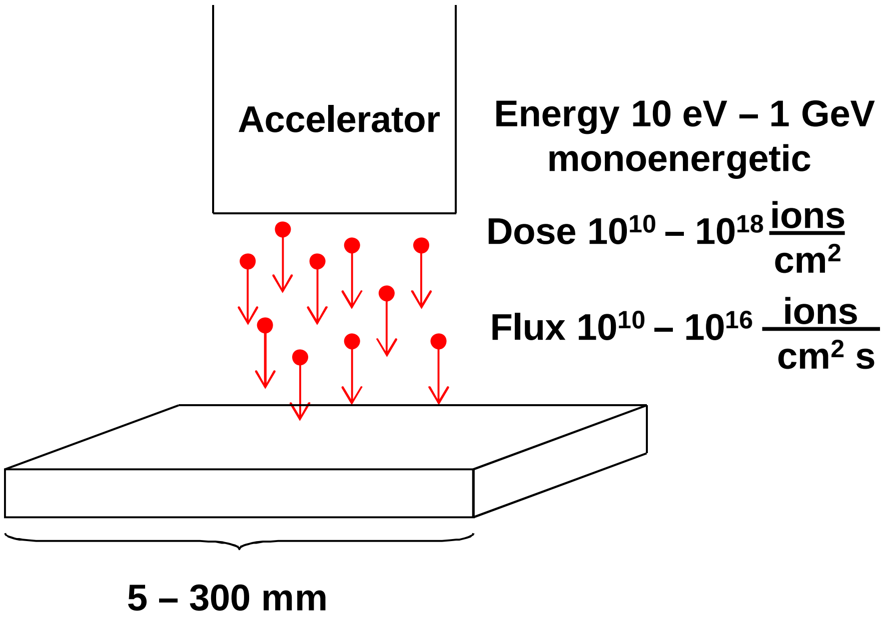
Main method of our groups: Molecular dynamics simulations

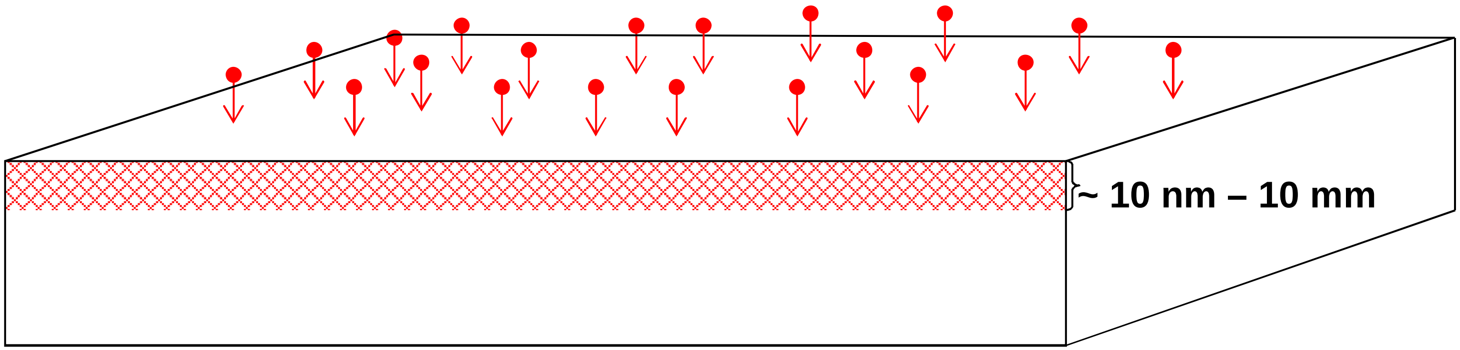
- Molecular dynamics = simulation of atom motion on computers by solving Newton's equations of motion numerically
  - Forces from interatomic potentials or quantum mechanics



Regular ion irradiation of materials

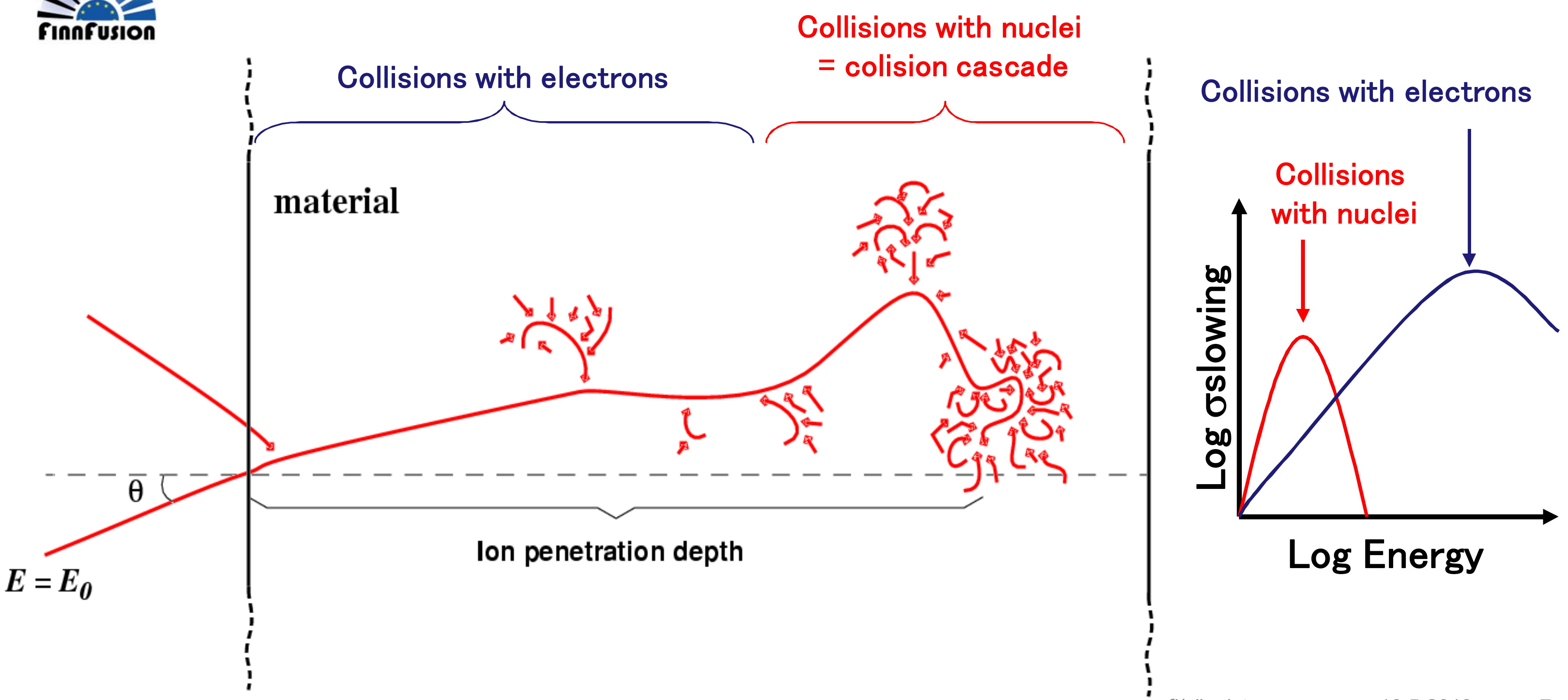
- Materials modification with ion beams: ions from an accelerator are shot into a material
- Huge (~ G€/year) business in semiconductor industry!
  - Doping of semiconductors
- Also big business for thin film production
- Extensively studied since 1950's or so.





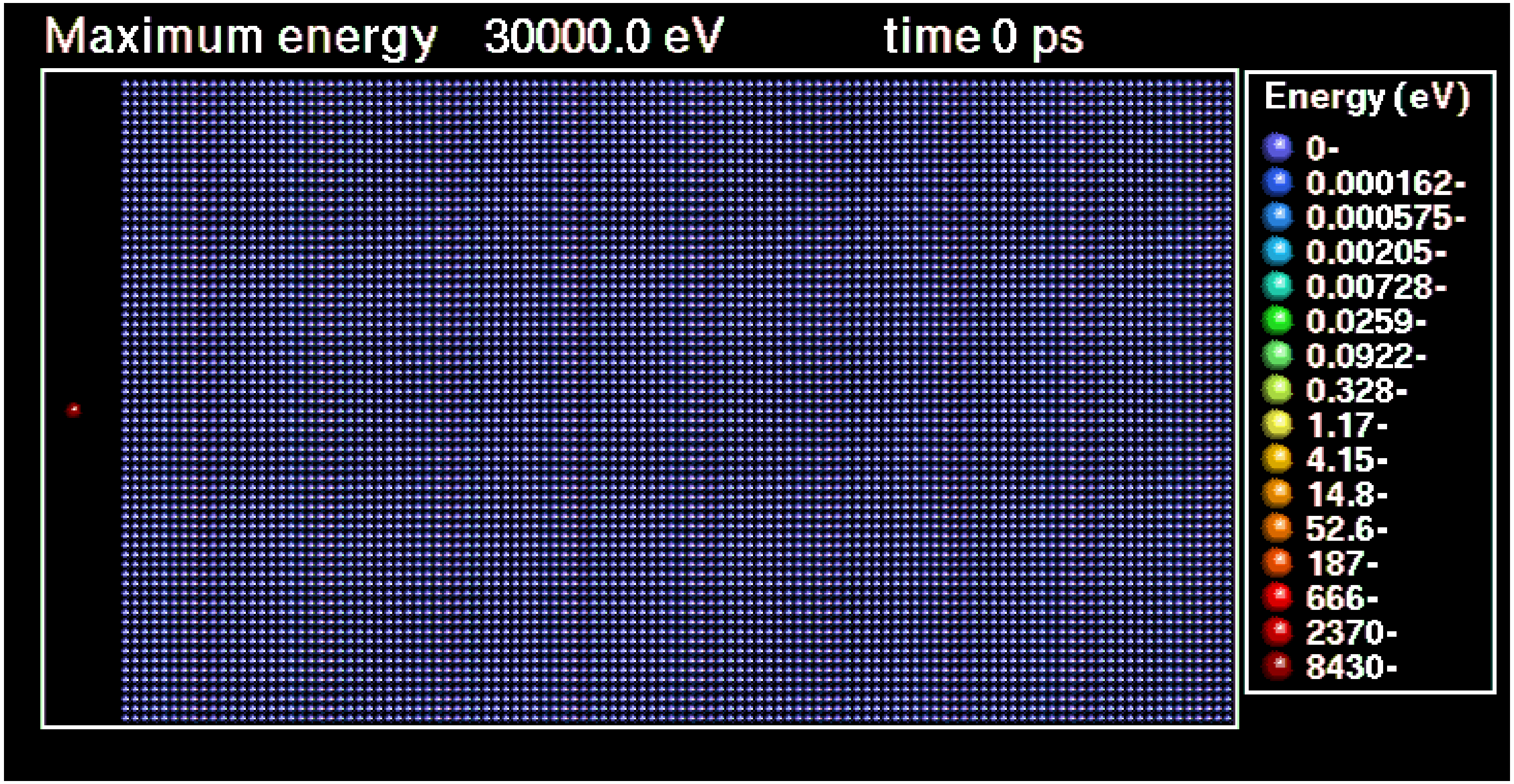
What happens when the ions enter the materials?

- Schematical illustration of the ion slowing-down process



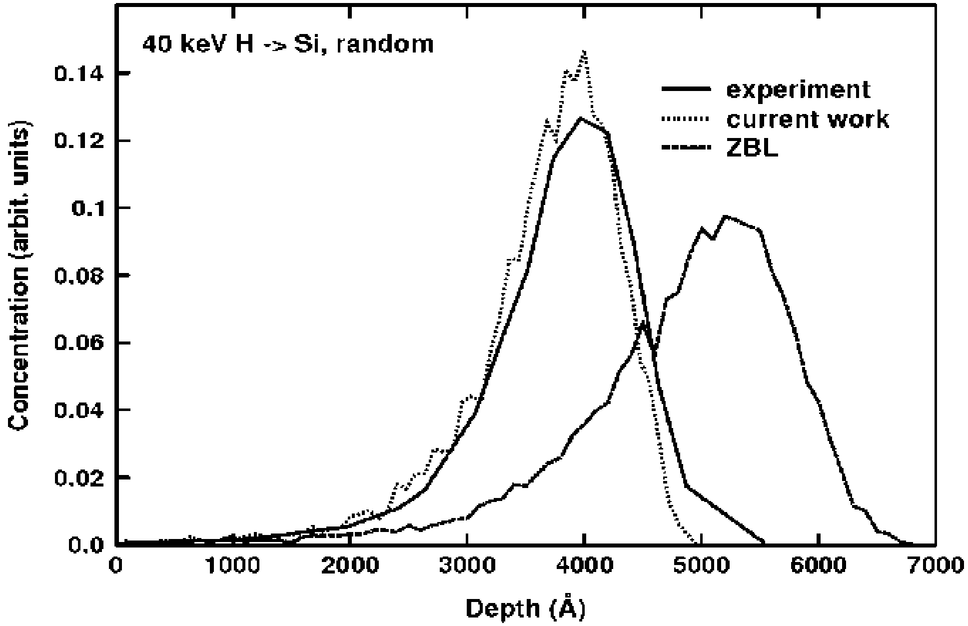
Molecular dynamics simulation of the collision cascade

- Model case: 30 keV Xe ion irradiation of Au



Outcome of regular ion implantation: implantation

- The base purpose of ion implantation is to obtain a dopant distribution at a desired depth in the material
- Typically slightly skewed Gaussian implantation profiles

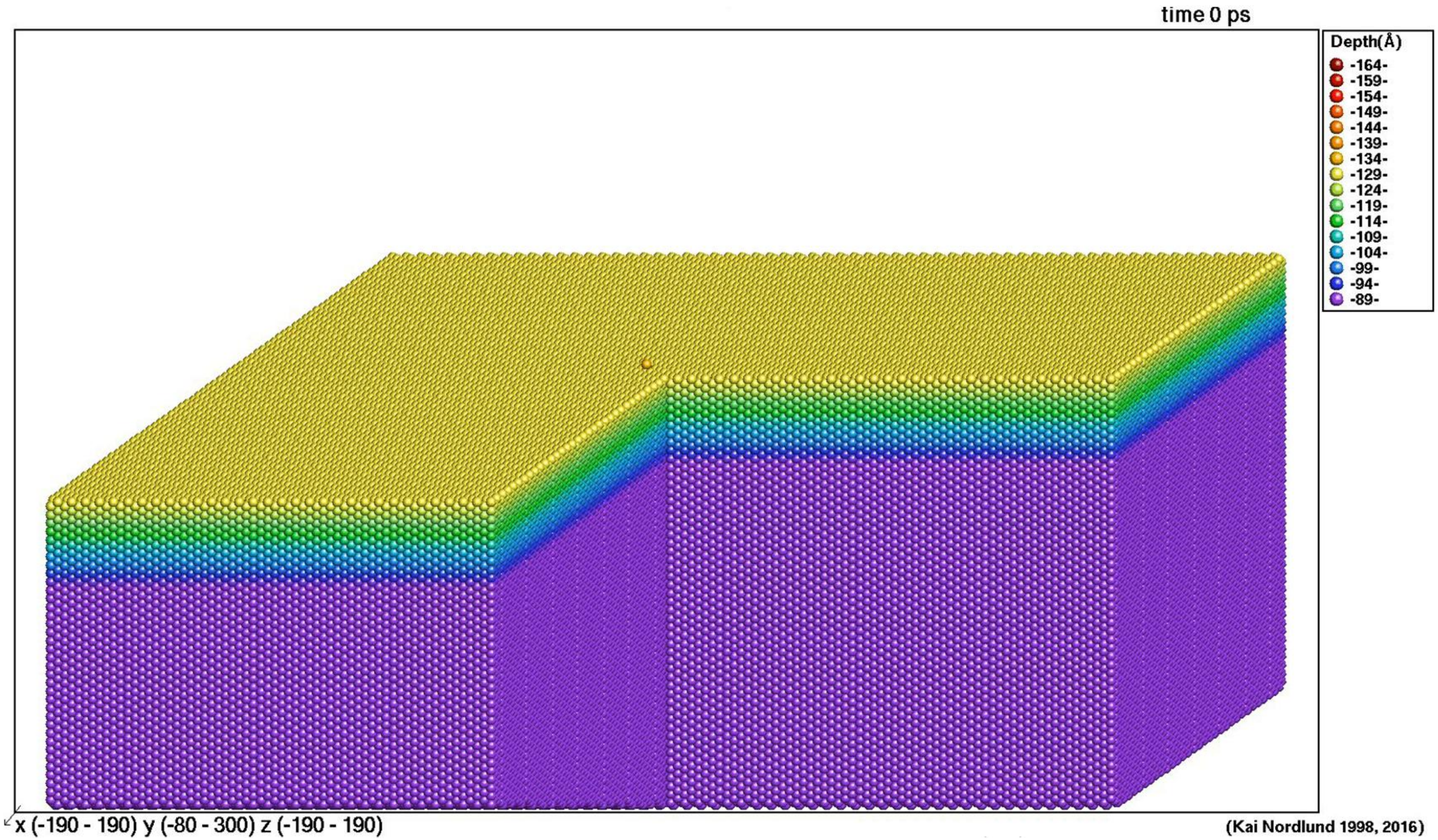


- Results from a special version of molecular dynamics that can efficiently simulate the range profiles
  - ”MD in Recoil Interaction Approximation”, MDRANGE code

[J. Sillanpää, K. Nordlund, and J. Keinonen, Phys. Rev. B 62, 3109 (2000); J. Sillanpää J. Peltola, K. Nordlund, J. Keinonen, and M. J. Puska, Phys. Rev. B 63, 134113 (2000); J. Peltola, K. Nordlund, and J. Keinonen, Nucl. Instr. Meth. Phys. Res. B 217, 25 (2003); J. Peltola, K. Nordlund, and J. Keinonen, Nucl. Instr. Meth. Phys. Res. B 212, 118 (2003)]

Outcome of regular ion implantation: cratering

- For heavy ions on dense materials, one often gets massive surface cratering effects
- Example: single 50 keV Xe ion on Au



[Nordlund, Physics World 2001]

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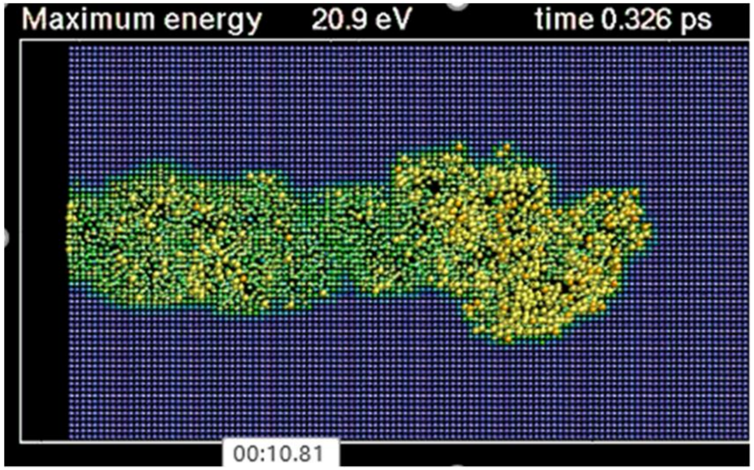
Fluxes

- Consider the typical ion beam fluxes and compare with the typical collision cascade
- Cascade area ~(10 nm)^2
- Cascade duration ~100 ps
- However, from flux **10^{16}** one can deduce that time between impacts in (10 nm)^2 area is 10 ms!
- Many orders of magnitude more than the cascade duration 100ps => collision cascades are normally completely independent of each other!

$$\textbf{Flux } 10^{10} - 10^{16} \frac{\text{ions}}{\text{cm}^2\ \text{s}}$$



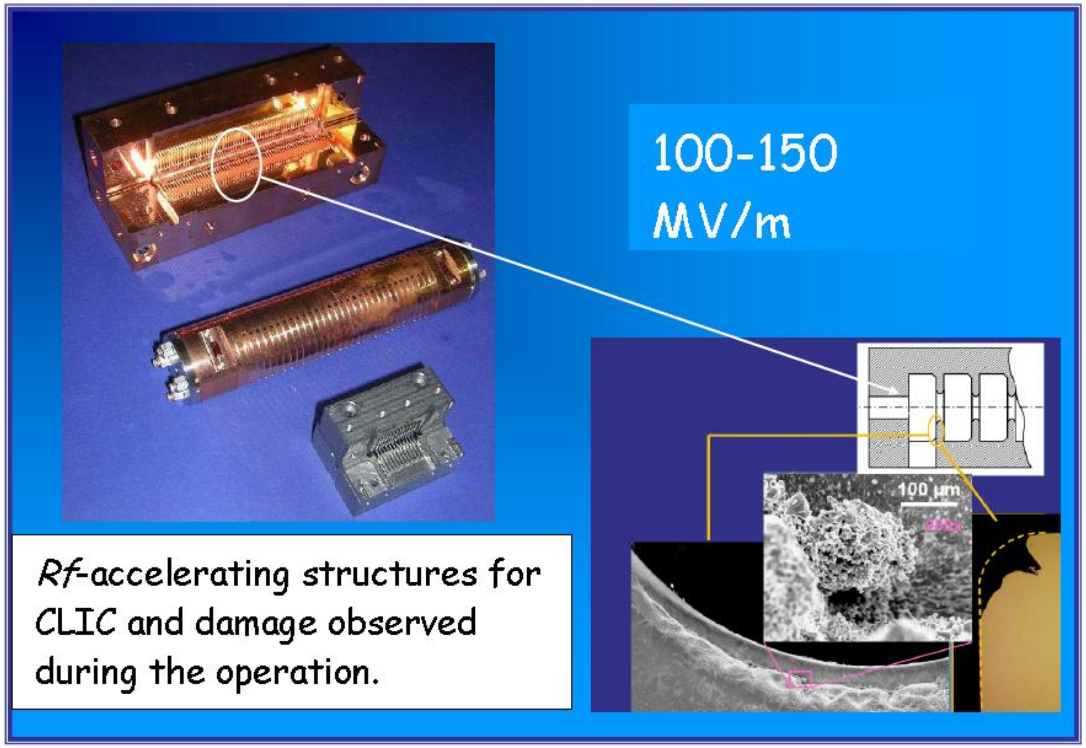
Possible laser acceleration applications for materials processing?

- Contrary to normal ion beams from conventional accelerators, laser accelerated ions have a high flux and broad energy profile

- **Two questions for rest of talk:**
  - **1. Can the very high fluxes be scientifically interesting, and do they occur anywhere else?**
  - **2. Could the broad energy profile be scientifically interesting?**

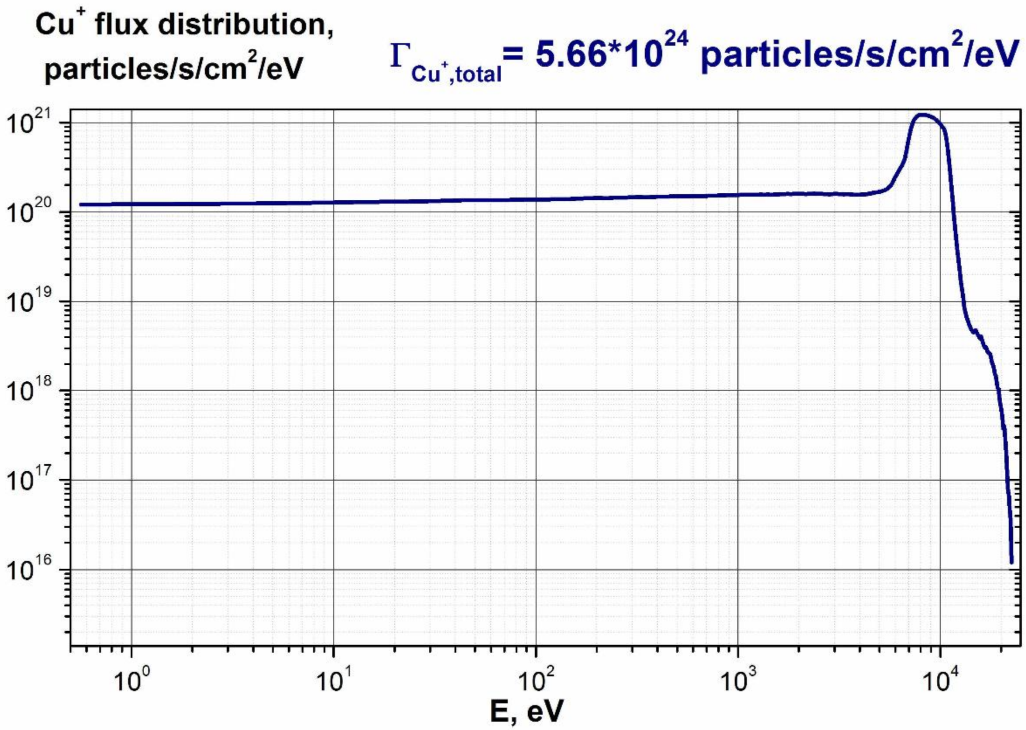
1. Very large fluxes: comparison with arc-plasma interactions with materials

- In high-accelerating-gradient accelerators, vacuum arcs often form spontaneously
- These have a massive effect on the materials around the arc



Fluxes in arcs

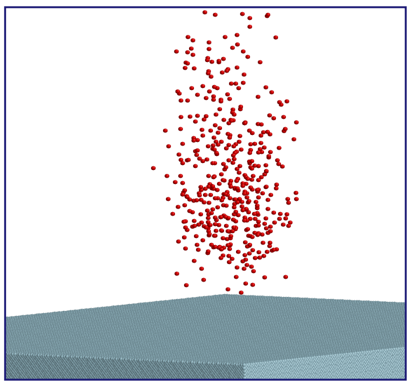
- For electrical arcs, particle-in-cell (PIC) plasma simulations show fluxes in arcs can be of the order of 10^{25} ions/cm^{2}s => time between impacts 10 ps => less than cascade lifetime!

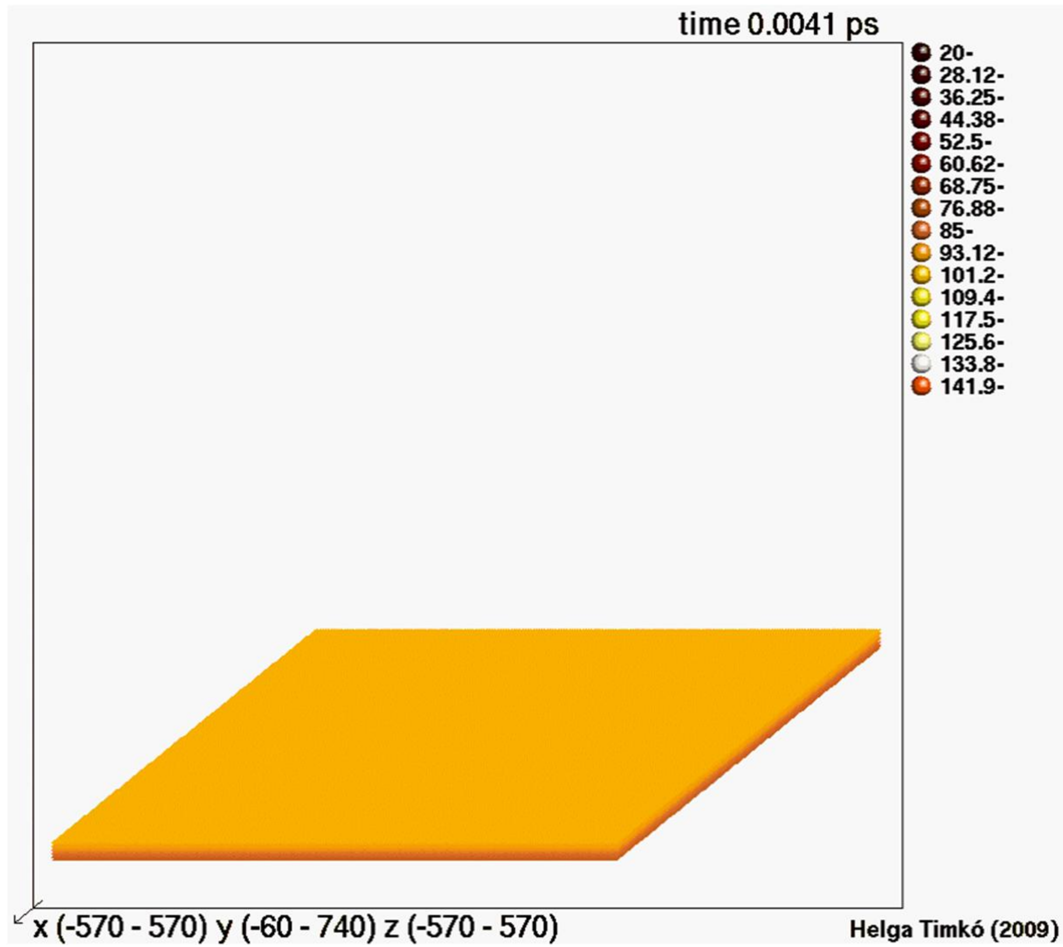


[H. Timko, F. Djurabekova et al, Phys. Rev. B **81**, 184109 (2010)]

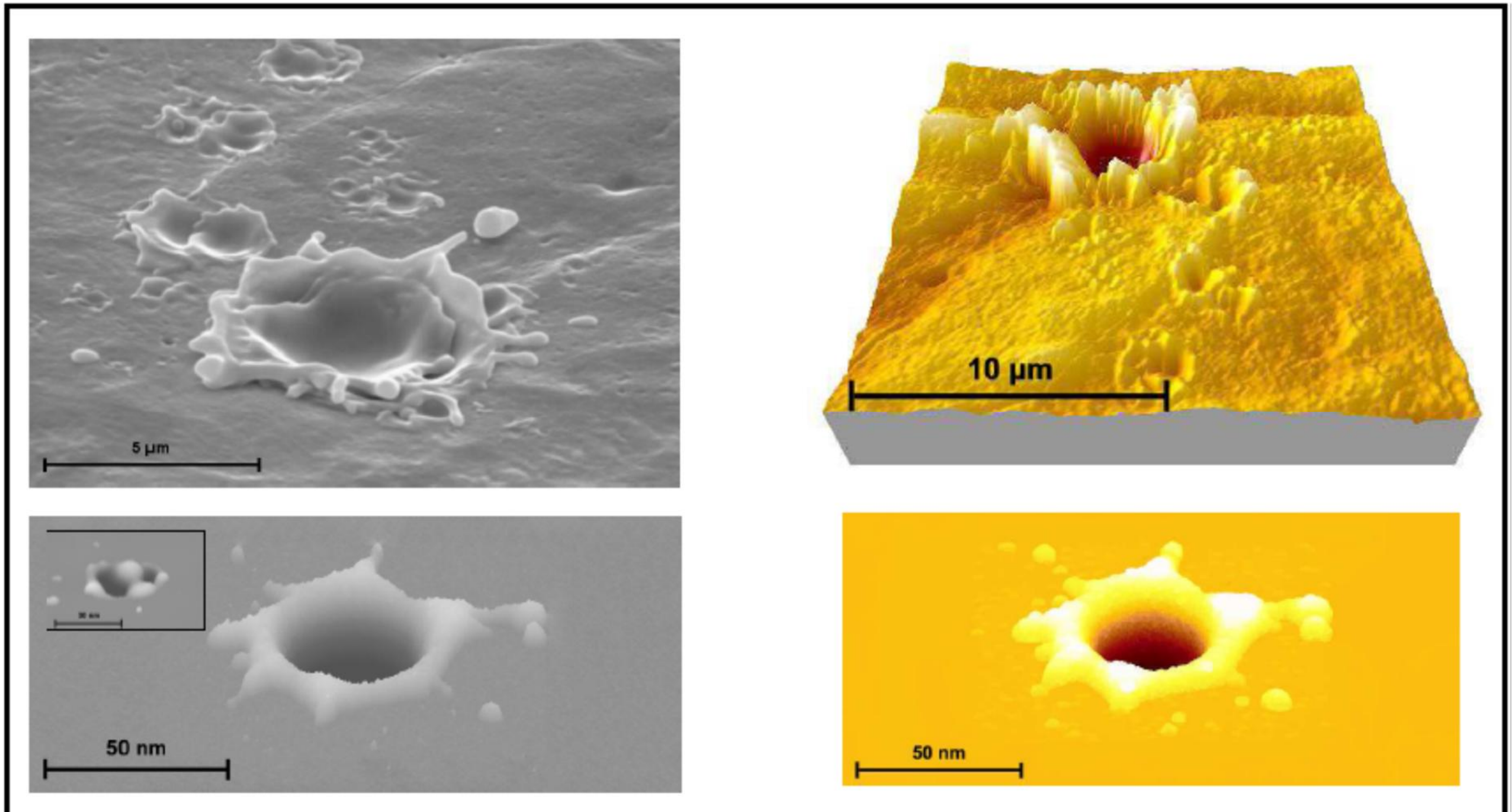
Simulation of arc irradiation: hundreds of cascades overlapping

- Top view of result on surface slice:



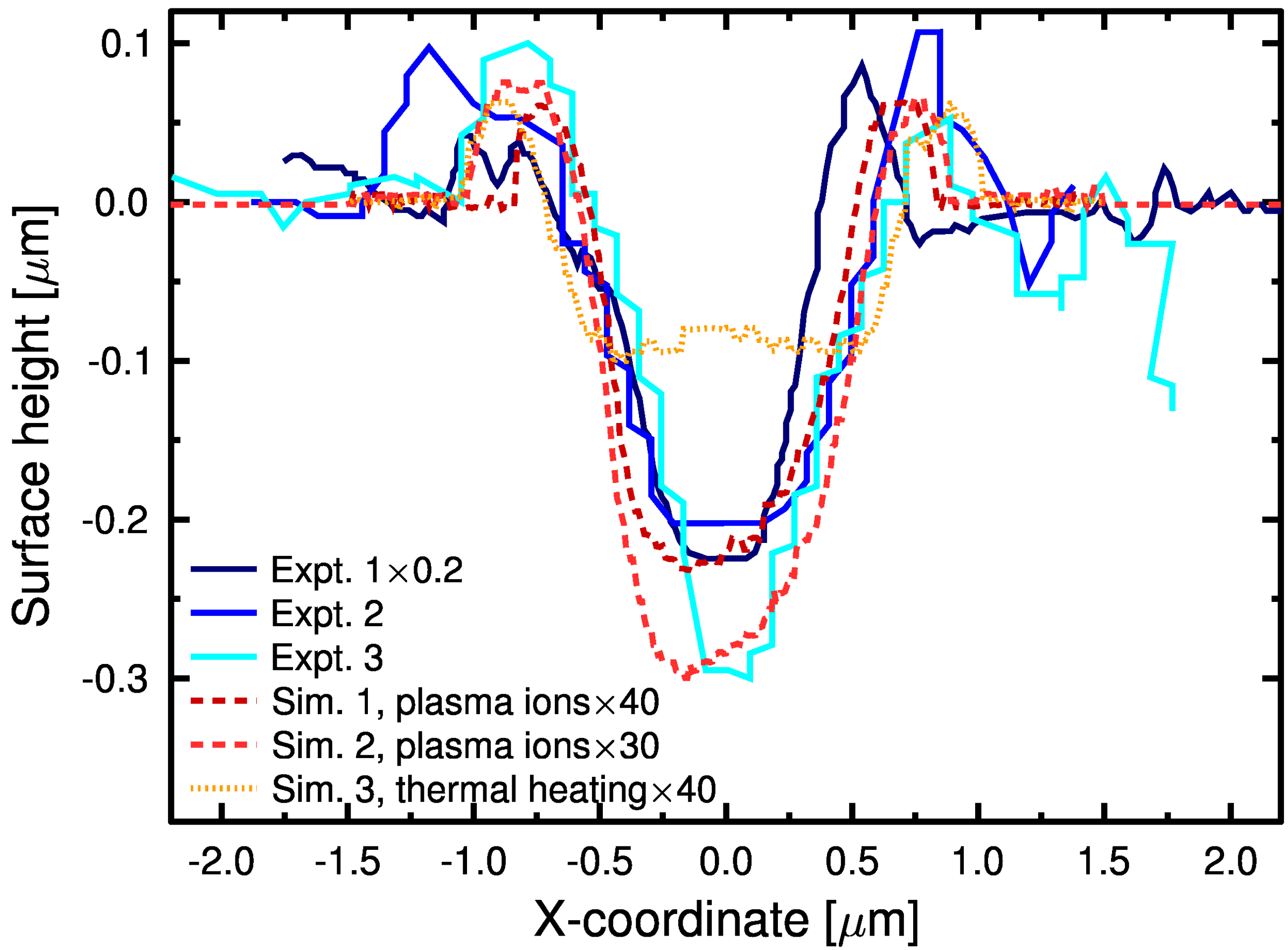


Comparison of crater shapes with experiments: qualitative



[H. Timko, F. Djurabekova et al, Phys. Rev. B **81**, 184109 (2010)]

Comparison of shapes with experiments: quantitative



[H. Timko, F. Djurabekova et al, Phys. Rev. B **81**, 184109 (2010)]

Laser acceleration relevance?

- Arc plasma irradiation makes for a new regime of ion beam physics: massively overlapping cascades
  - Very interesting from a basic science point of view
- However, arc plasmas are **very** uncontrollable (initiation is explosive and random), making doing both the science and application of them challenging
  - Systematically lowering flux not possible

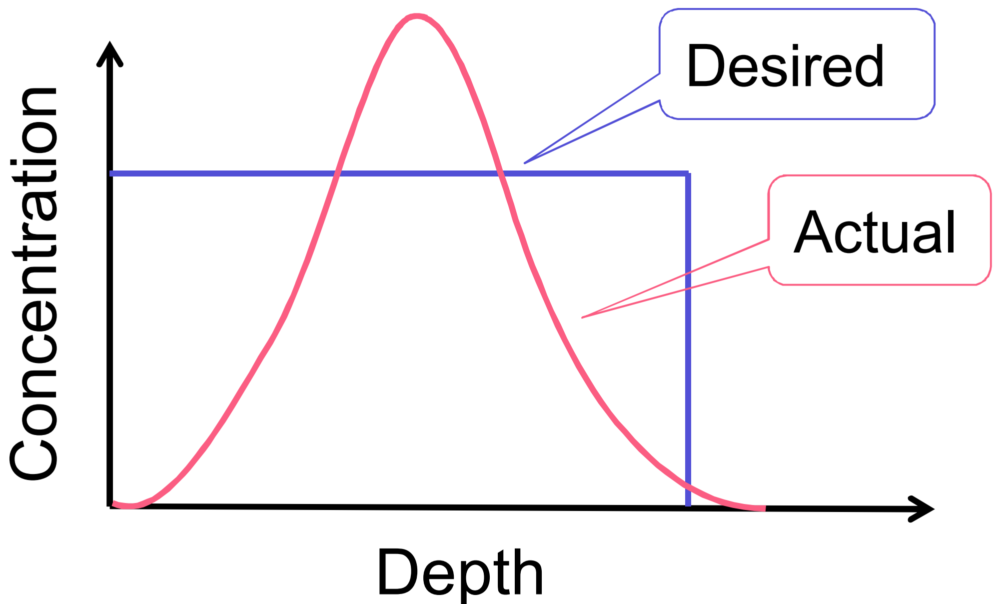
- High-flux laser accelerated ions could be very interesting for studying radiation effects in the overlapping cascade regime
  - Initiation control perfectly controllable
  - Flux control also possible (?)

Laser acceleration benefits

- The laser-acceleration could have the advantage over arcing that one could use any ion-material combination
  - Arcing is limited to using the same material for both the implanted ions and the material to be implanted.
- Also a regime slightly below the “heat spike overlap” regime could be very interesting from a basic science point of view
  - It would allow studying materials modification in a regime where there is very little time for thermally driven defect migration.
  - The balance between direct damage production clustering and migration-induced clustering is something of a hot issue in the field now
- The combination of very high flux density and little time for defect migration could allow for making new kinds of metastable thin films.

2. Box-like implantation profiles?

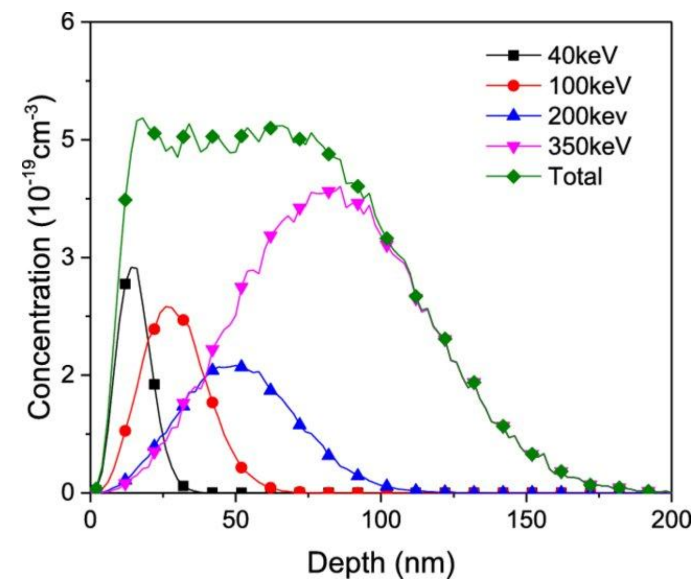
- The normal ion implantation leads to ~ Gaussian profiles
- However, for a simple semiconductor design, it would usually be desirable to have a box-like dopant distribution



Multi-energy implants

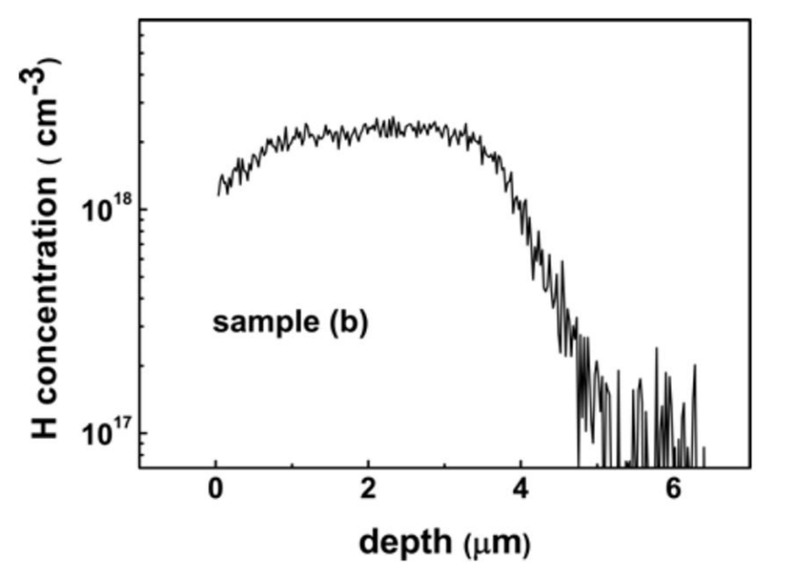
- To get somewhat box-like profiles, it is possible to do many implants at different energies and fluences, so that the total concentration profile is somewhat box-like
- Example: 4 energies to get close (simulation)

Simulation: In -> ZnO, 4 energies



[Yaqoob and Ming, J. Appl. Phys. 120 (2016) 115102]

Experiment: H -> Zn0, 5 energies

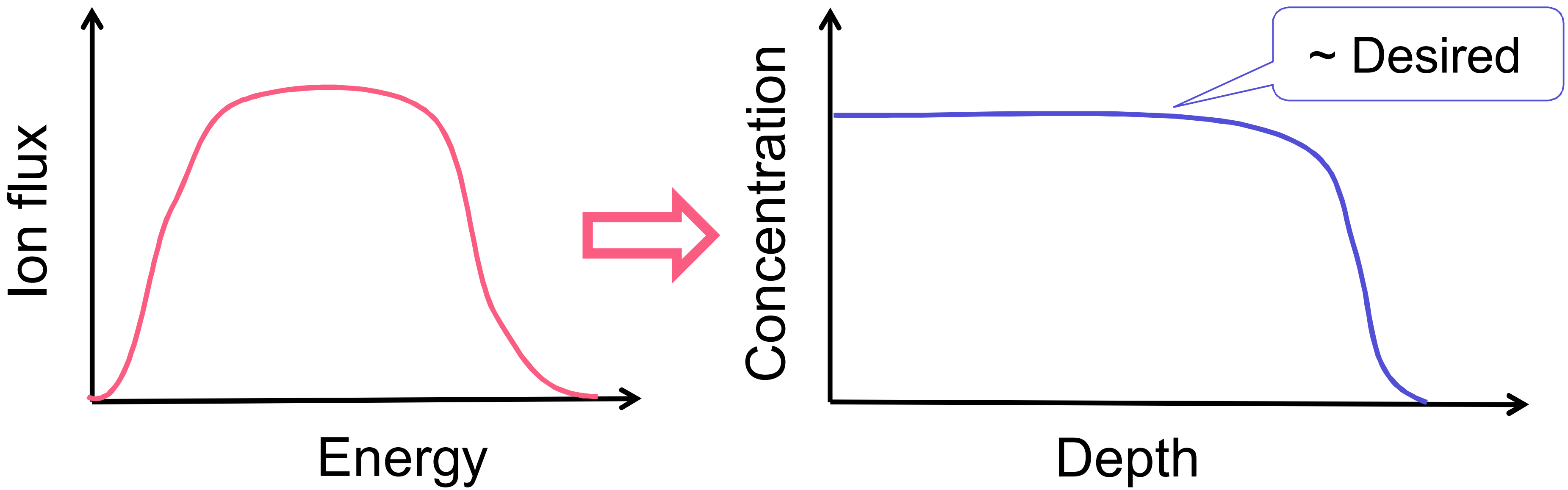


[Schifano et al, phys. stat. sol. (a) 205 (2008) 1998]

[Achieving box-like profiles is also of industrial relevance: **https://www.axcelis.com/knowledge-center/damage-engineering-purion-xe-high-energy-ion-implanter; Damage Engineering on Purion XE High Energy Ion Implanter;** By J. DeLuca et al, Axcelis Technologies, Inc.]

Box-like profiles

- Could laser-driven acceleration achieve it in a single step!?
  - Careful control of energy profile should enable this



- Is it possible to achive this level of control with laser acceleration??

Summary; these and potential other uses?

	Ion energy range and distribution	Flux (ions/m^2 s)	Type of ion	Irradiation area	Expected outcome and relation to other fiels
2.	keV's, but with limited energy spread	<< 10^{27}	Any	Broad beam	Efficient ion implantation with box-like dopant profiles; potential use in semiconductor technology
	keV's	< 10^{27}	Any	Any	Material modification with limited defect mobility; way to test diffusion/flux effects on ion materials modification.
1.	100 of eV's to keV's	≥ 10^{27}	Heavy	Focused	Local cratering; way to test arc plasma modification of materials
	keV to MeV's	≥ 10^{27}	Medium or heavy	Broad beam	Ablation of material; analogy to laser ablation
	> 10's of MeV's	≥ 10^{27} (including electrons)	Heavy	Focused	Track formation; analogy to swift heavy ion irradiation. Synergy effects of ions and electron material modification.

[Nordlund and Djurabekova, ALPA book (2018)]

Conclusions

- Laser particle acceleration could be:
  - Very interesting to study extreme flux effects on materials in a more controllable way than electric arcing
  - Potentially an interesting way to make box-like ion implants??
  - Also other applications
- In general, laser particle acceleration can open up a new regime of ion irradiation physics to study!