ION-INDUCED CHANGES ON SOLIDS WITHIN APPA EXPERIMENTS FAIR

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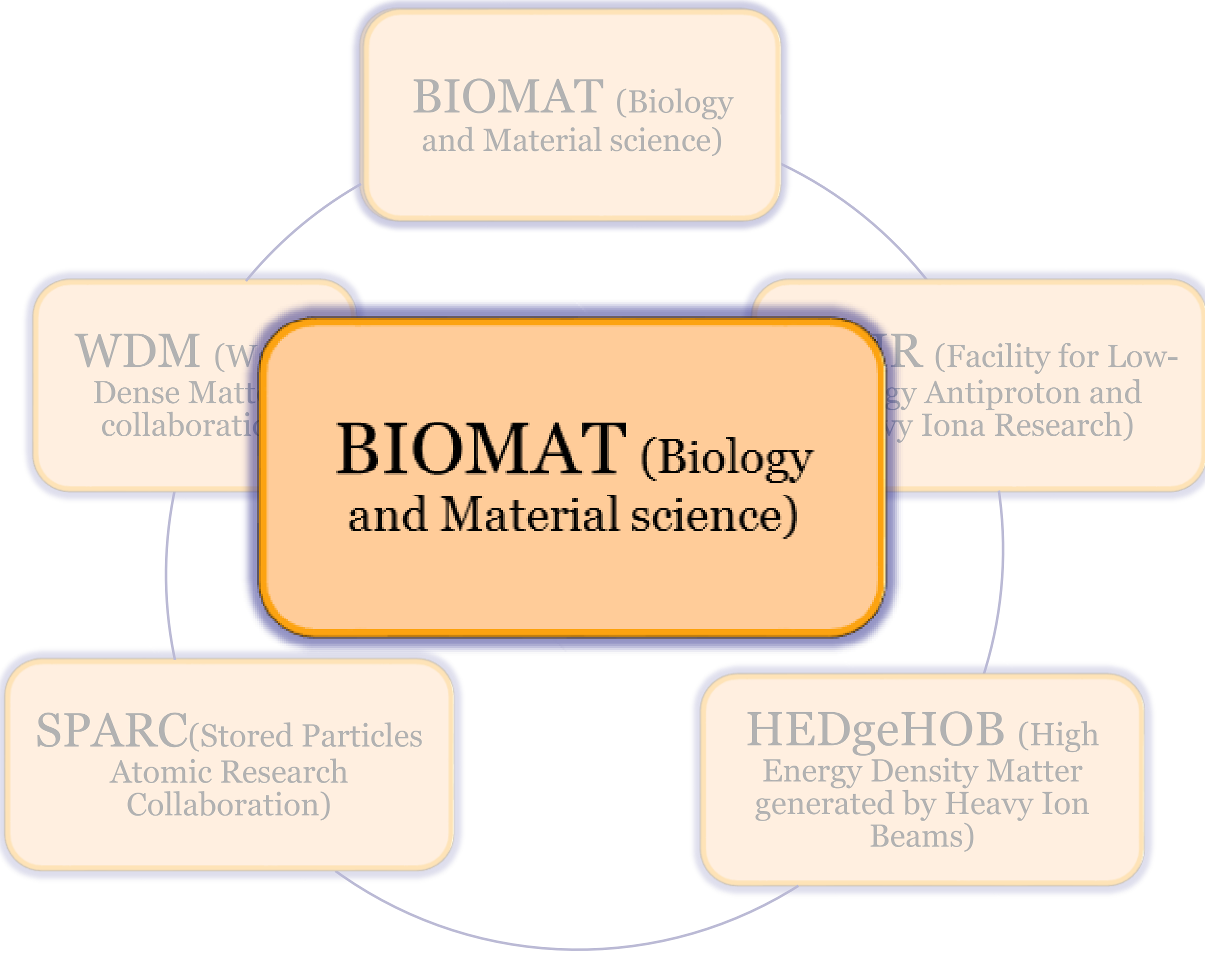
Ex perimental (and not only) collaborators

- **C. Trautmann, GSI (Germany)**
- **M. Tomut, GSI (Germany)**
- **M. Schleberger, Univ. Duisburg-Essen (Germany)**
- **O. Ochedowski**
- **J. Kotakoski, Univ. Of Vienna (Austria)**
- **A. Krasheninnikov, HRDZ (Germany)**
- **S. Daraszewicz (**theory, *TTMD model***), UCL (UK)**

APPA Physics - Atomic, Plasma Physics and Applications

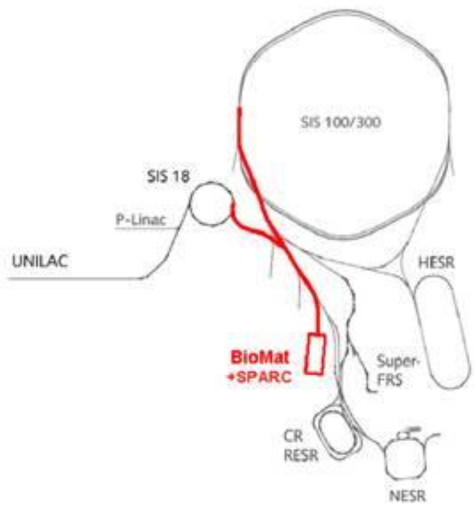


BIOMAT

High-Energy Irradiation Facility for Biophysics and Materials Research

Biophysical experiments

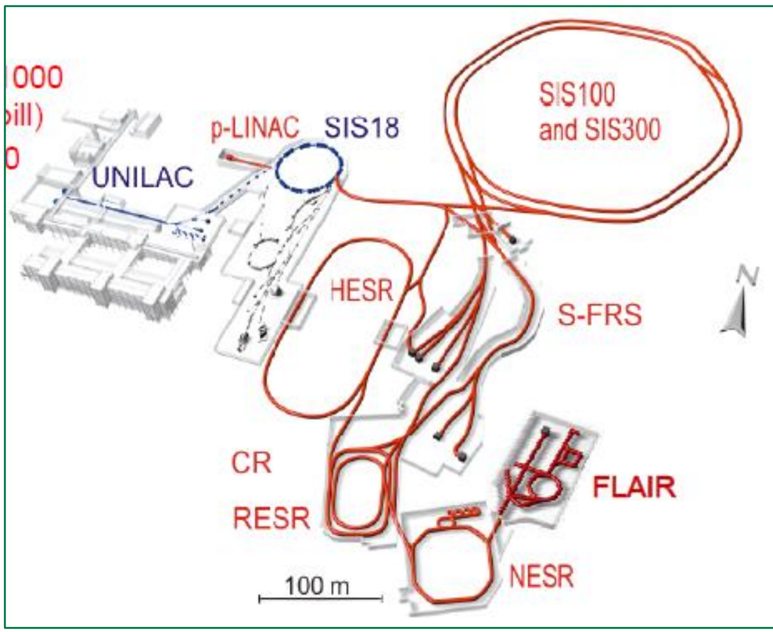
Experiments for ion-induced changes in solids

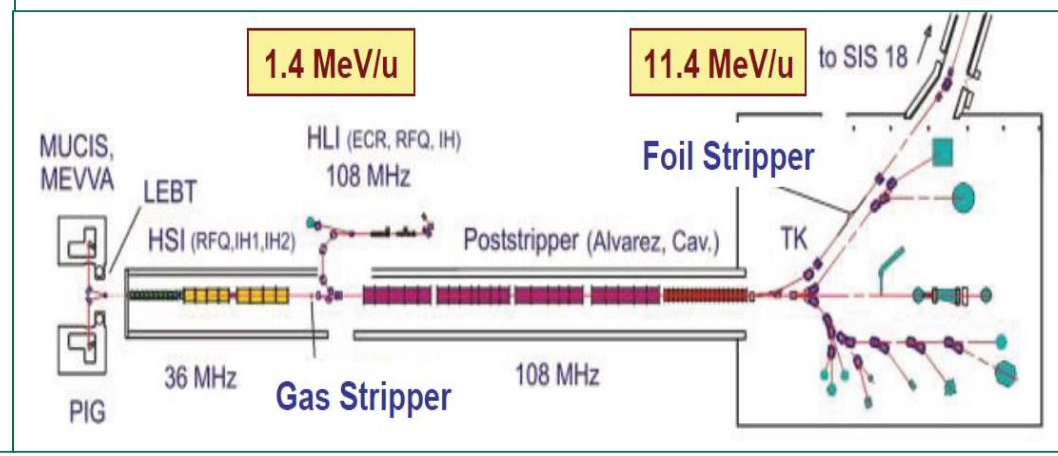


- The FAIR accelerator complex at GSI will be a facility, where heavy ions with energies up to 10 GeV can be used for radiobiology and materials research.

Focus within FAIR

- Our collaborators are the GSI staff, who was and is involved with the heavy-ion UNILAC linear accelerator





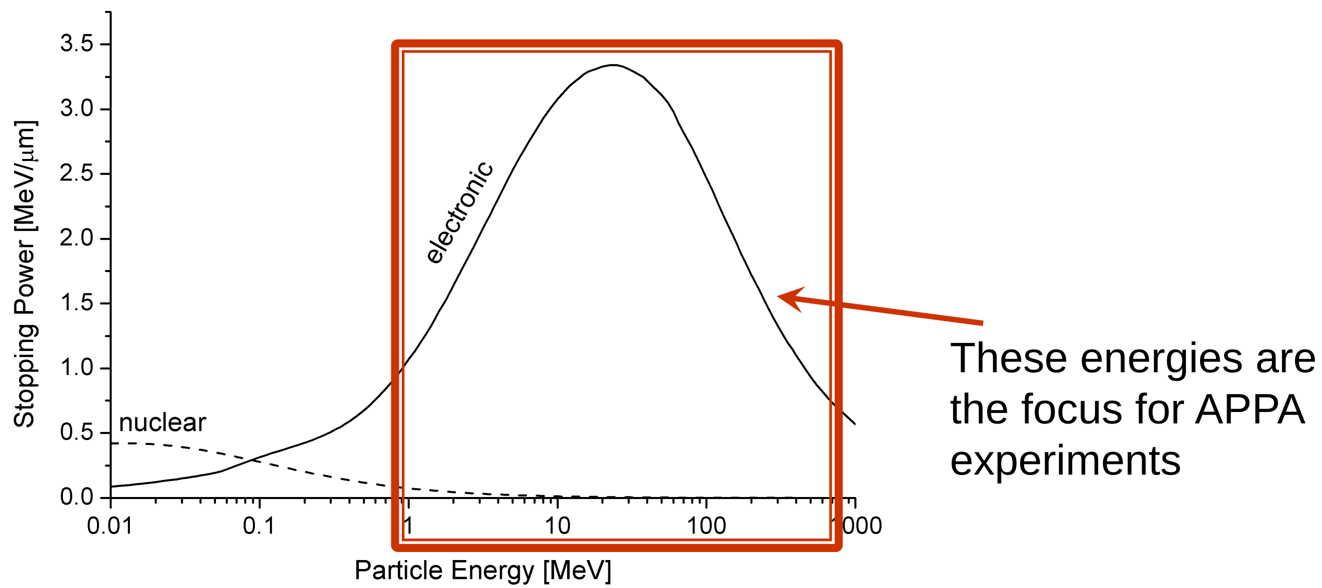
Charge stripping foils at GSI

Different carbon foils irradiated with different ions to the same fluence, but pulsed and quasi-continuum beams, comparison made at FAIR/GSI.

- Amongst the most recognized candidates for future foils are diamond-like carbon (**DLC**), amorphous carbon (**a-C**) with the different level of porosity, graphene (**Gr**) platelets-based carbon (**GPBC**) and carbon nanotube (**CNT**) networks.
- To reduce the effect of the foil material on the incoming ion beam, the density of the stripping foils must be kept low. For LINAC the density of carbon foils are exceptionally low, approx. 20 – 30 μg/cm². The tested foils usually last only few minutes before the failure, although the produced in GSI laboratory a-C foils were able to last up to several hours.

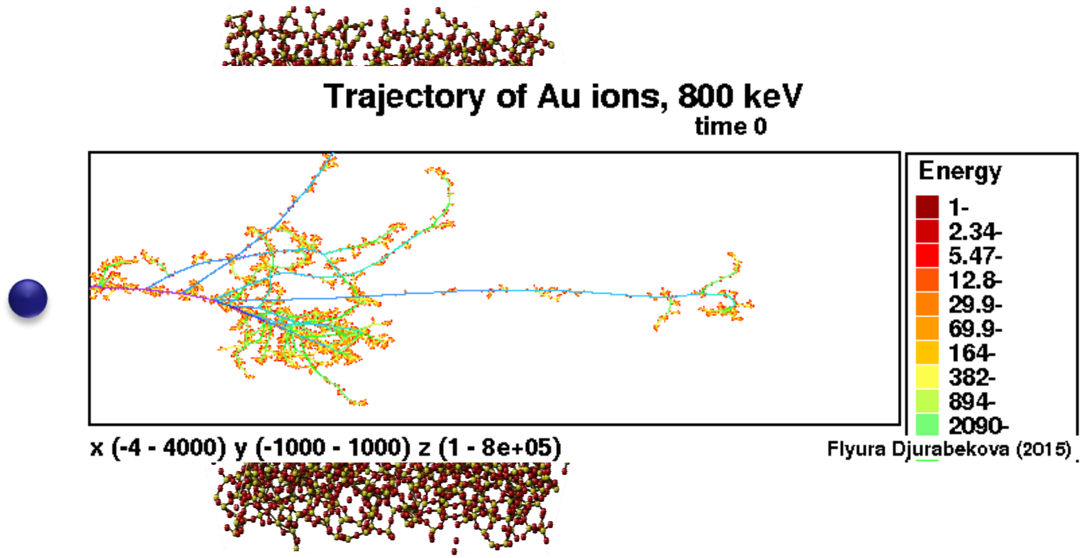
What do we study? Radiation effects in materials

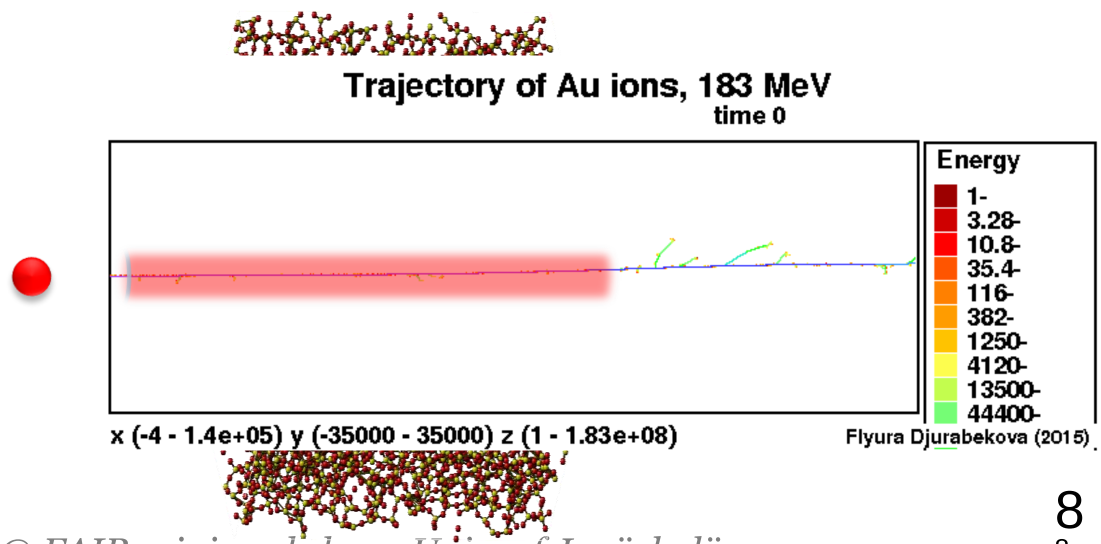
- Radiation effects due to ion irradiation in materials are traditionally considered separately in two energy regimes:
  - < 1 MeV/amu – nuclear collisions are important
  - ≥ 1 MeV/amu – electronic effects are important



Two regimes of irradiation

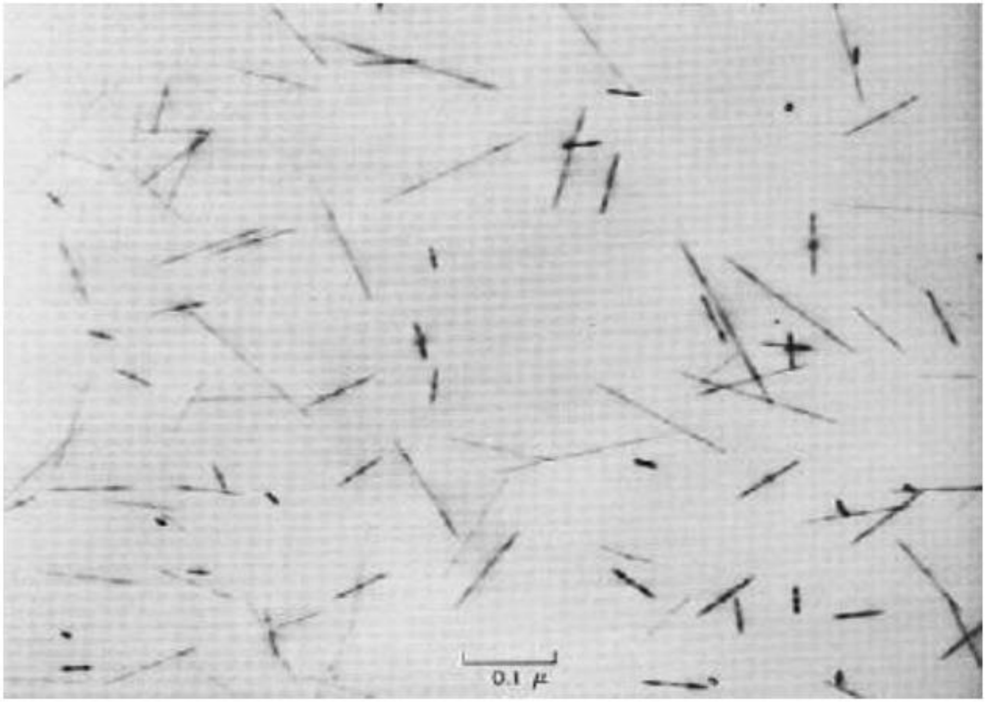
- Low/medium energy of ions causes many atomic collisions.
- With the increase of ion energy, the probability of atomic collisions is decreasing





Experimental evidences

- Ion tracks are seen as regions of structural transformation in the wake of passing ion



Latent tracks in mica
E. Silk and R. Barnes, Acta Metallurgica 9, 558 (1961)

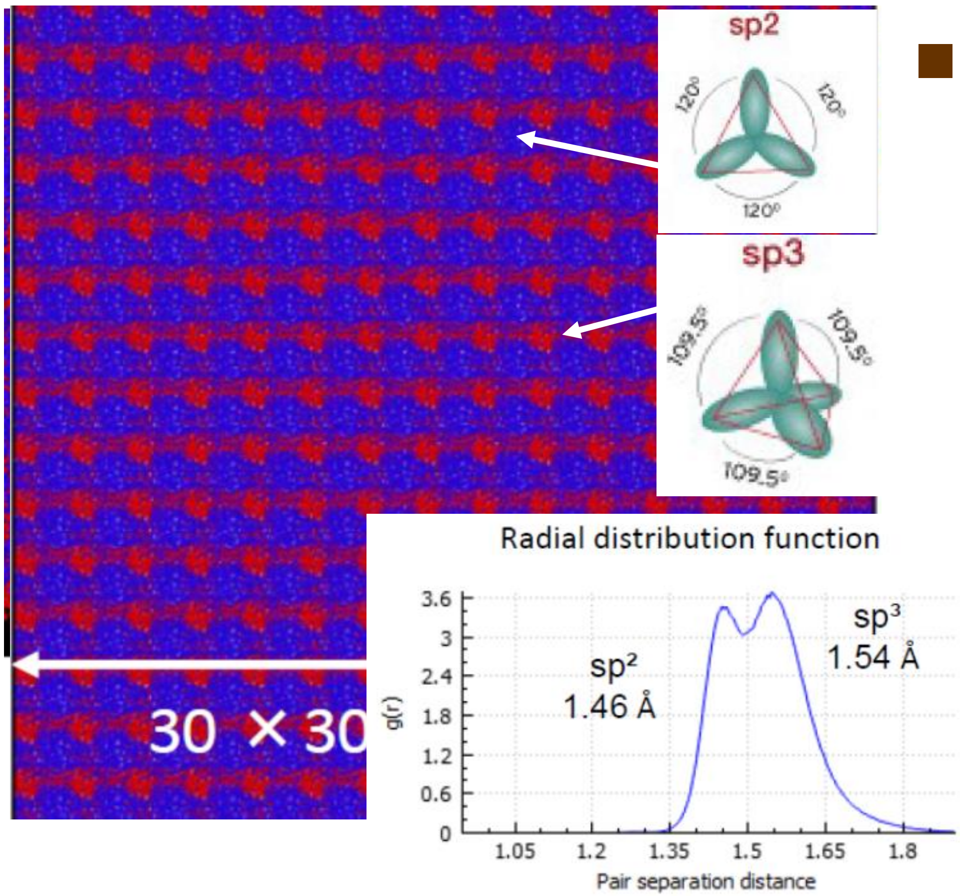
Swift Heavy Ion tracks in matter

- Swift (E_{kin}/mass ≥ 1MeV/amu) Heavy ($\mu \geq 40$ amu) Ion tracks are regions of structural transformation left behind by the ion
- They can be used in number of applications
  - making filters, biosensors, fission track dating…
  - Construct the efficient charge stripping foils to be used for he nuclear applications

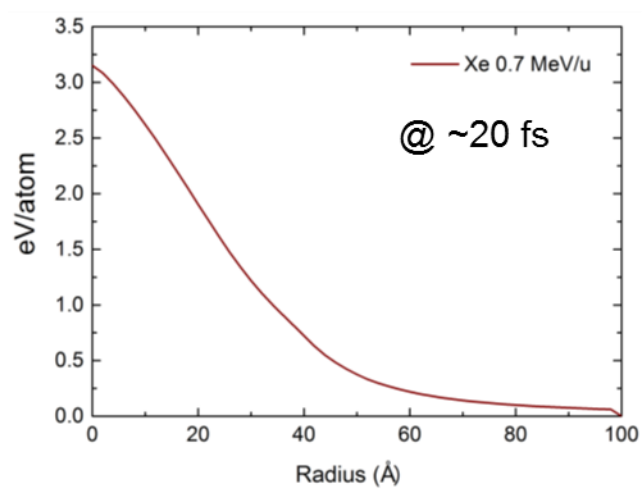
Different carbon foils irradiated with different ions to the same fluence, but pulsed and quasi-continuum beams, comparison made at FAIR/GSI.

SHI irradiation of a-C

- a-C was constructed by quenching from the melt (0.1 K/fs) with the number of atoms corresponding to 60% sp^2



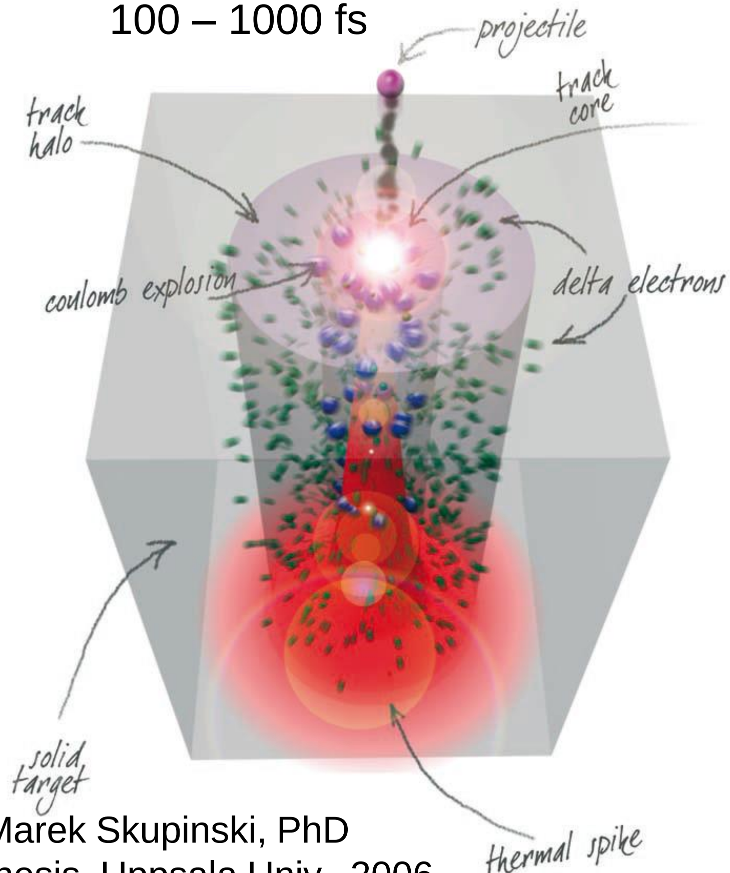
- The prepared sample was irradiated with Xe ions with 91 MeV ions (0.7 MeV/) by using the inelastic thermal spike model



How do tracks form?

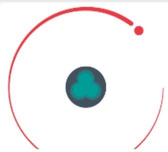
- The swift heavy ion knocks out keV range electrons
- The initial distribution of excitations can be calculated using cross sections from optical measurements
- This can be fitted by empirical formulae to obtain the initial energy deposition

Time interval of initial collisions:
0.01 - 0.1 fs
Time for atoms to relax:
100 – 1000 fs



Marek Skupinski, PhD thesis, Uppsala Univ., 2006

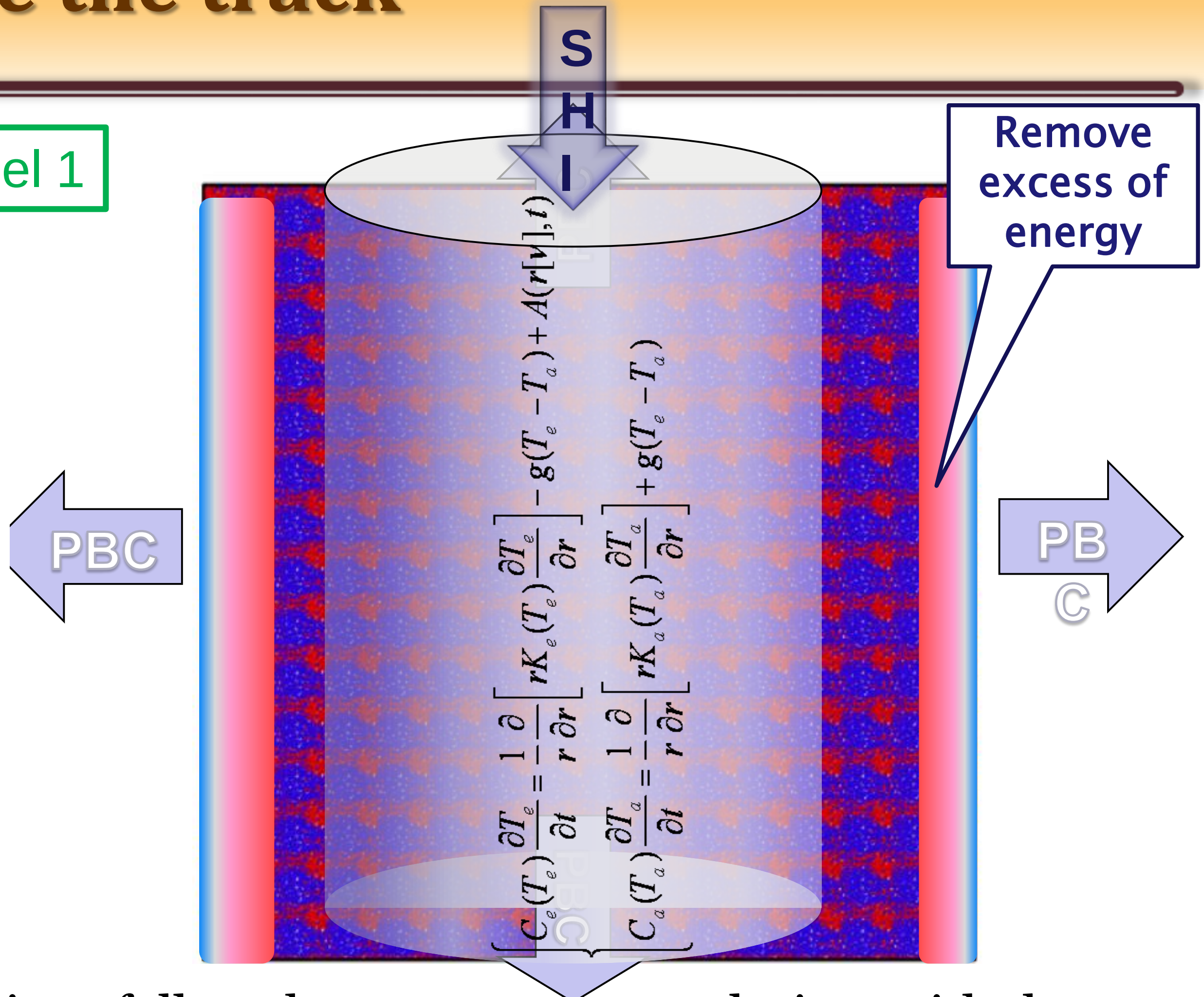
Inelastic thermal spike model to simulate the track



Model 1

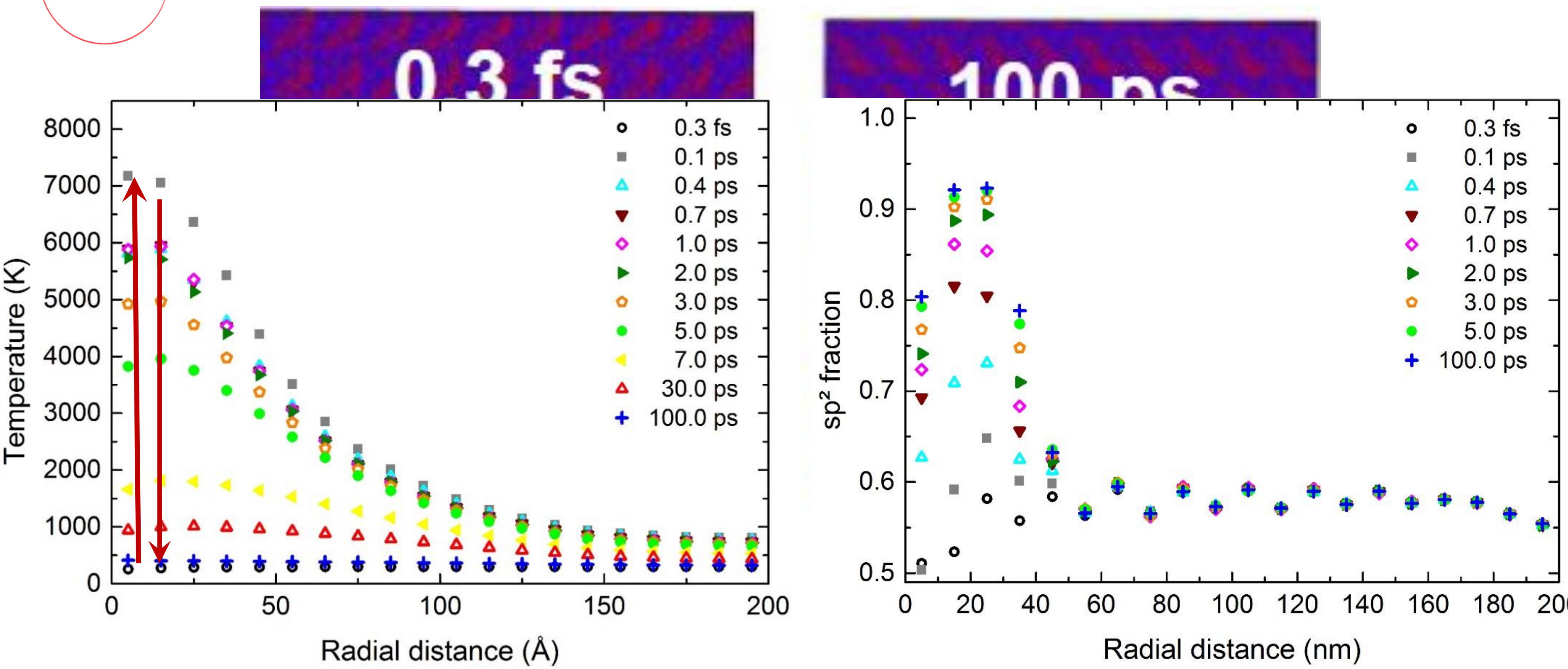
MD + heat spike or MC model

- Get forces $\mathbf{F} = -\nabla V^*_i(\mathbf{r}^{(n)})$ and $\mathbf{a} = \mathbf{F}/m$
- *Solve:* $\mathbf{r}^{(n+1)} = \mathbf{r}^{(n)} + \mathbf{v}^{(n)}\Delta t + {}^1/_2\,\mathbf{a}\,\Delta t^2 + \ldots$; $\mathbf{v}^{(n+1)} = \mathbf{v}^{(n)} + \mathbf{a}\,\Delta t + \ldots$
- Modify velocities: $\mathbf{v}^{(n+1)} = \mathbf{v}^{(n+1)} + \mathbf{v}^*_i(S_e,t)$
- Move time forward: $t = t + \Delta t;\ n = n+1$
- Repeat



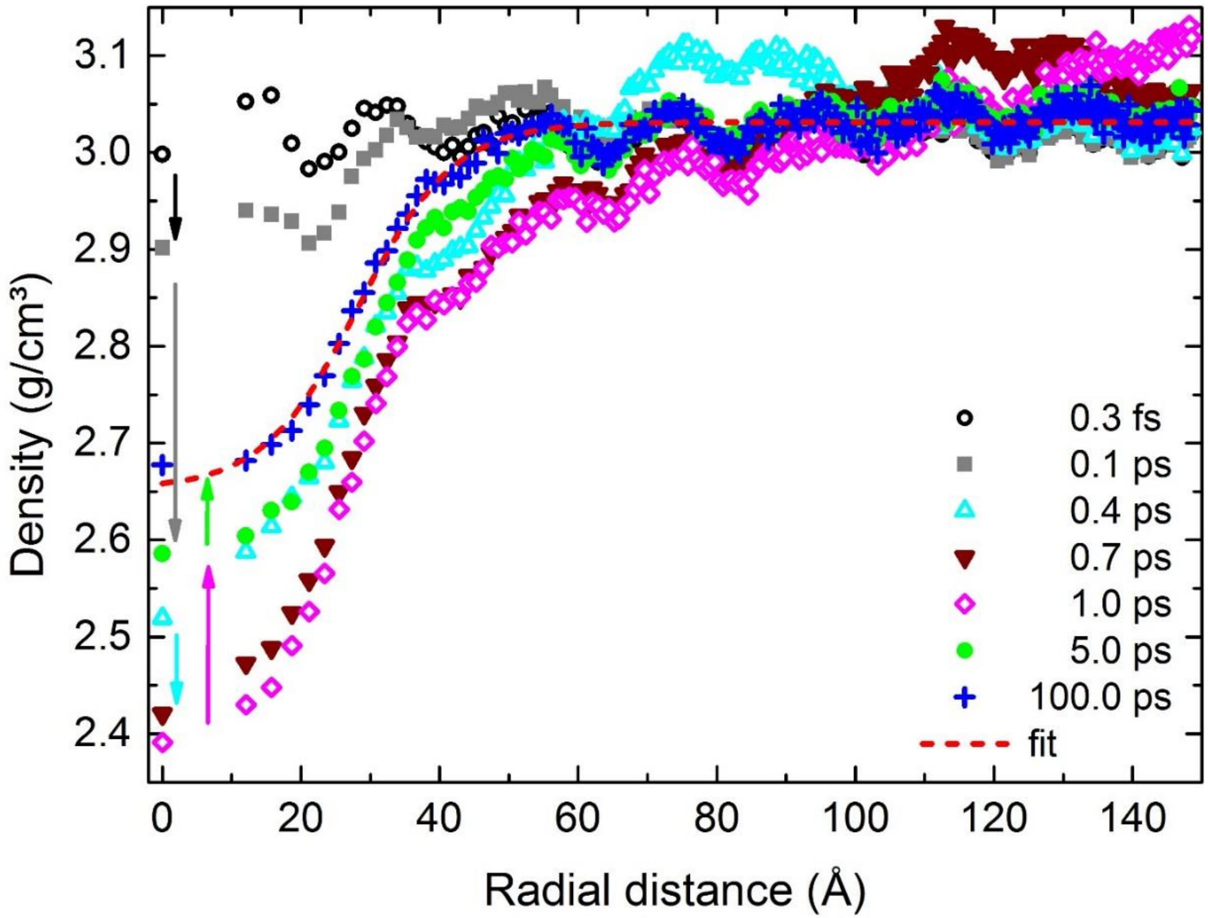
- 0 - 500 ps MD simulations follow the temperature evolution with the atomistic view on phenomena like mass transfer, pressure waves, phase transitions etc. in the material

Temporal evolution of a track in a-C



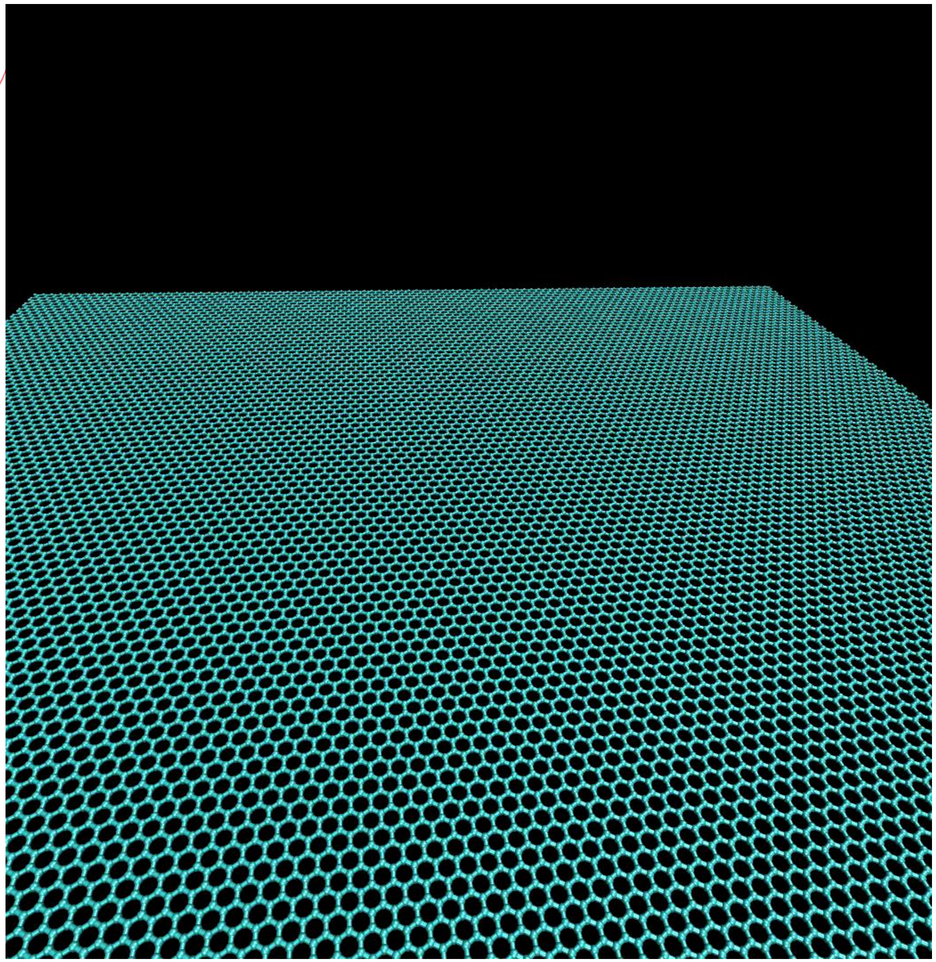
- Time evolution of temperature and corresponding change of sp^2 fraction during the swift heavy ion impact as a function of radial distance from the track center.

Density evolution in the track



- A clear core with the lower density (3 nm in radius) is formed after the impact.

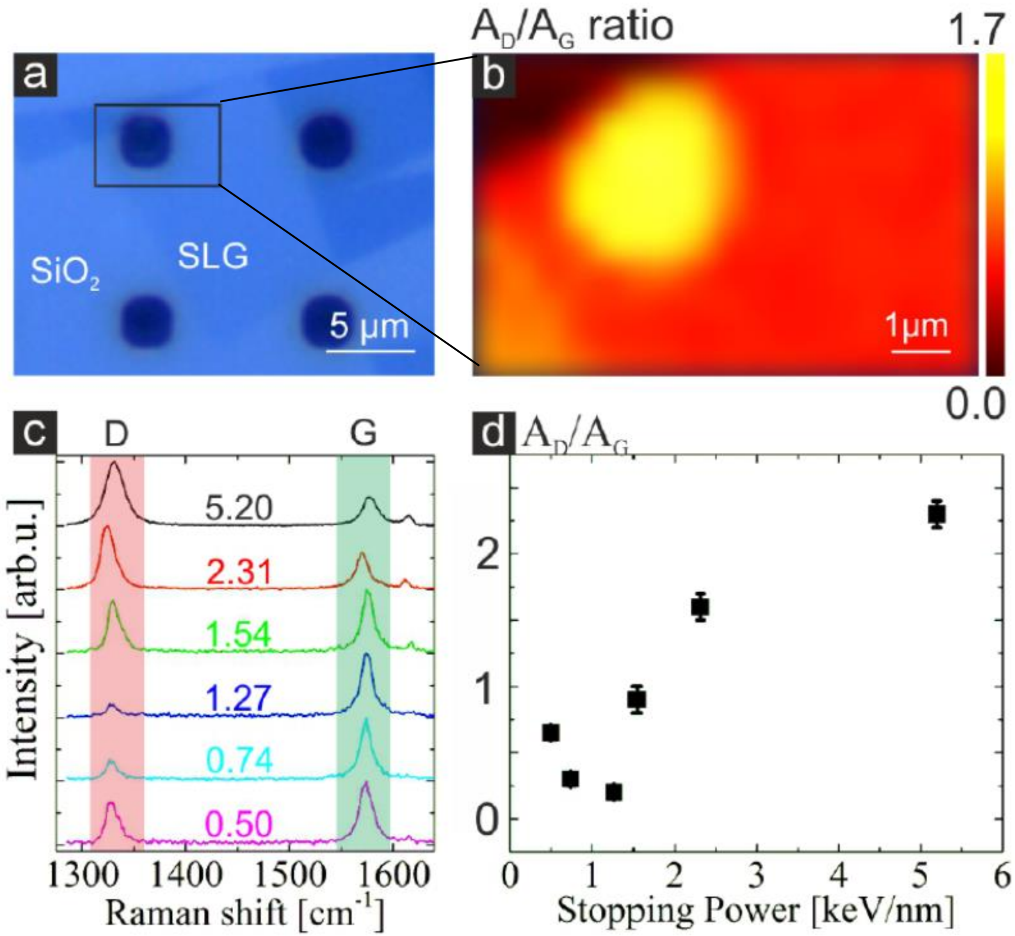
Simulation of track formation in graphene by Ta 84 MeV



- Big number of atoms is sputtered, some are trapped at the edges of the forming pore.
- Lots of wobbling

E. Harriet Åhlgren,
Univ. Of Helsinki

Raman spectrometry of SHI irradiated graphene

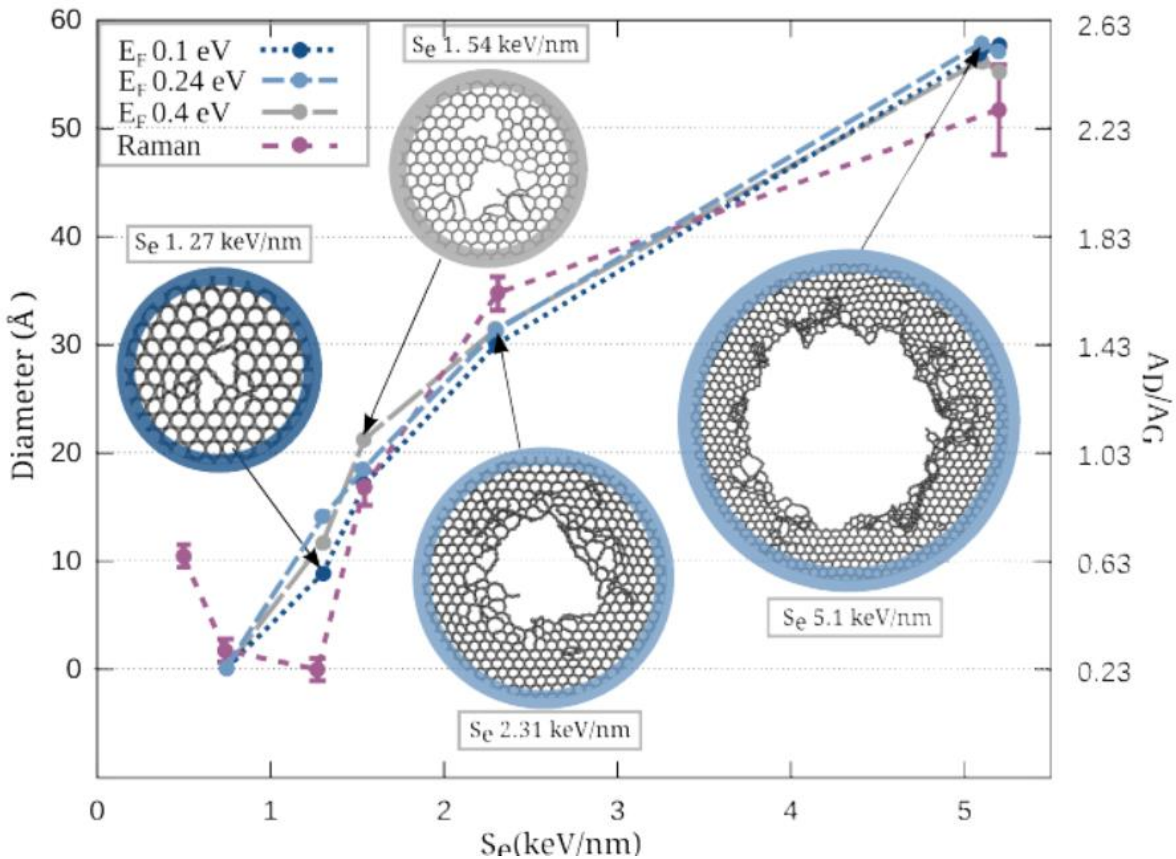


ion	E [MeV]	S_e [keV/nm]
O	1	0.5
O	3	0.74
Si	6	1.27
Si	15	1.54
I	23	2.31
Ta	84	5.10
Xe	91	5.20

Experiments by Oliver Ochedowski and Marika Schleberger, DEU.

- Experimental results show the increase of the damage with the energy

Threshold of pores formation in suspended graphene



- Results do not depend strongly on the dopant level and agree well with Raman spectrometry results (K_e=450 $Wm^{-1}K^{-1}$). Threshold for damage production is slightly lower in MD simulations.

Summary

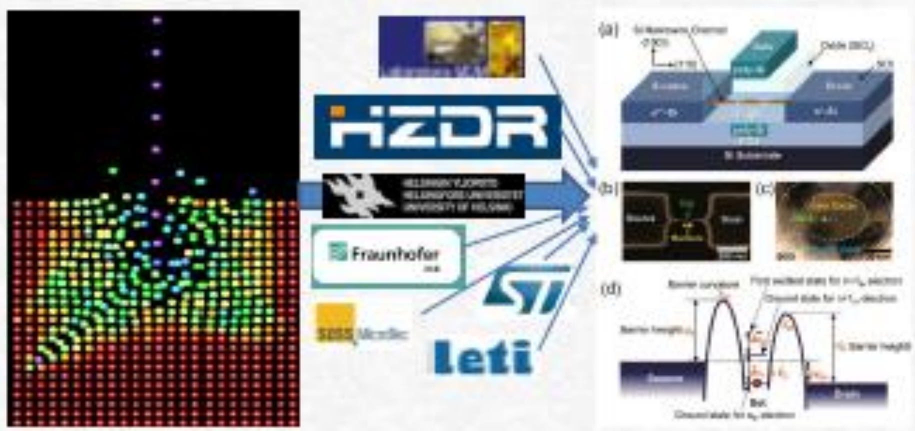
- In amorphous carbon materials, the effect of swift heavy ion, resulting in a inelastic thermal spike, clearly leads to graphitization of the core of the track
- Two temperature molecular dynamics model is able to capture the main processes ongoing during the SHI irradiation of graphene:
  - The model predicts the formation of stable damage of graphene at the energy loss threshold similar to one derived from the experiment.
  - The size of the pores depends on the thermal conduction, which is poorly defined experimentally as well.

26.11.2015

PhD student position in ion beam physics
EU project

The Materials physics simulation groups (Prof. Kai Nordlund and Adj. Prof. Flyura Djurabekova) at the Department of Physics, University of Helsinki have an opening for a PhD student position in the field of atom-level classical molecular dynamics simulations of an ion implantation process for synthesizing single-electron transistors. The work is part of an EU project "IONS4SET" lead by the Helmholtz-Zentrum Dresden-Rossendorf. The simulation part of the project is to be done in Helsinki with close collaboration with the 6 European partners.

The friendly working environment is created by the large international (about 30 members) and very active (more than 40 international refereed publications annually) closely collaborating materials physics simulations groups of Prof. Kai Nordlund, Docents Antti Kuronen and Flyura Djurabekova http://beam.acclab.helsinki.fi/sim. In addition to carrying out active independent research, the groups have a broad range of international contacts with leading ion beam, fusion research, and accelerator technology groups around the world, including the Big Science research activities at CERN, EUROFusion, and FAIR.



The position is intended primarily for an student with a MSc completed or close to completion in physics or a closely related discipline. The position can be filled from Feb 1, 2016 for a duration of 2+2 years. The PhD work, fully paid at a starting level of about 2200 EUR/month, will also involve enrollment in the MATRENA doctoral programme and taking 60 ECTS credits in physics and transferable skills.

The applicants should have a good track record of studies in physics and programming skills. Experience in graphical programming is considered a plus.

If interested, send a CV and M. Sc. or B. Sc. study credit certificate to Adj. Prof. Djurabekova, flyura.djurabekova@helsinki.fi

Spring E-MRS 2016
Lille - France
May 2-6

www.emrs-strasbourg.com

http://www.european-mrs.com/2016-spring-symposium-bb

Symposium BB: Defect-induced effects in nanomaterials

Topics:

* Effects of grain boundaries and interfaces on the diffusion and transport processes in nanomaterials.
* Swift heavy ion irradiation as the means to tailor nanomaterials
* Electronic structure of defects in nanostructures; consequences for carrier transport, magnetism, optical and electronic properties, as well as device parameters.
* Creation, evolution and properties of radiation defects in nanosize materials and heterostructures; the role of interfaces, nonstoichiometry, strain and adjacent layers.
* Defects in two-dimensional materials.
* Multiscale computer modeling of defect creation in nanomaterials.
* Novel technological processes of micro-, nano- and optoelectronics using defects and radiation effects in nanostructures.

Chairpersons:

- ***Eugene Kotomin***, University of Latvia
- ***Flyura Djurabekova***, Univ. of Helsinki, Finland
- ***Nikolai A. Sobolev***, Univ.de Aveiro and I3, Portugal
- ***Yanwen Zhang***, ORNL, UT, USA
- ***Mark C. Ridgway***, Australian National University

Thank you for your attention!