Experimental studies and multiscale modeling of latent tracks in radiation-resistant insulators

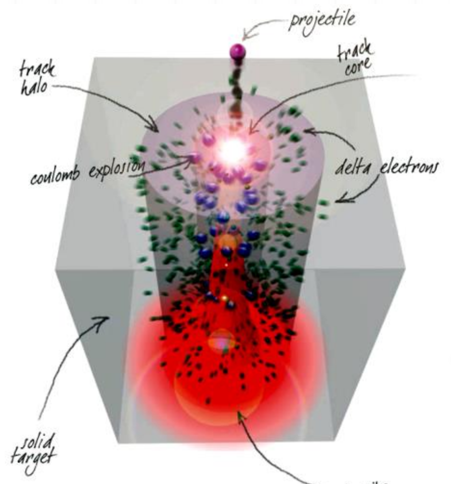
FLNR JINR
V.A. Skuratov, R. Rymzhanov, A.E.Volkov, A.Ibrayeva, N.S.Kirilkin

Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic
N.Medvedev

Centre for HRTEM, Nelson Mandela University, Port Elizabeth, South Africa
J.H.O'Connell, A. Janse van Vuuren, J. Neethling.

Institute of Nuclear Physics, Nur-Sultan, Kazakhstan
M.V.Zdorovets

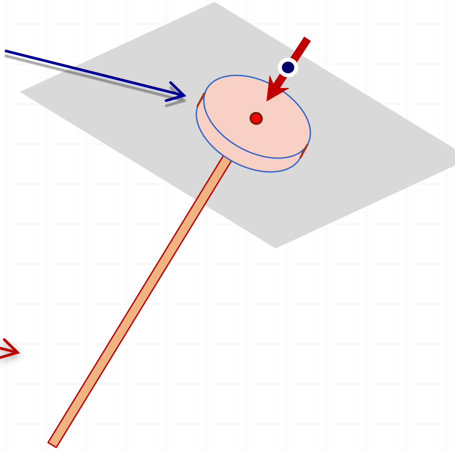
SHI track: temporal and spatial scales

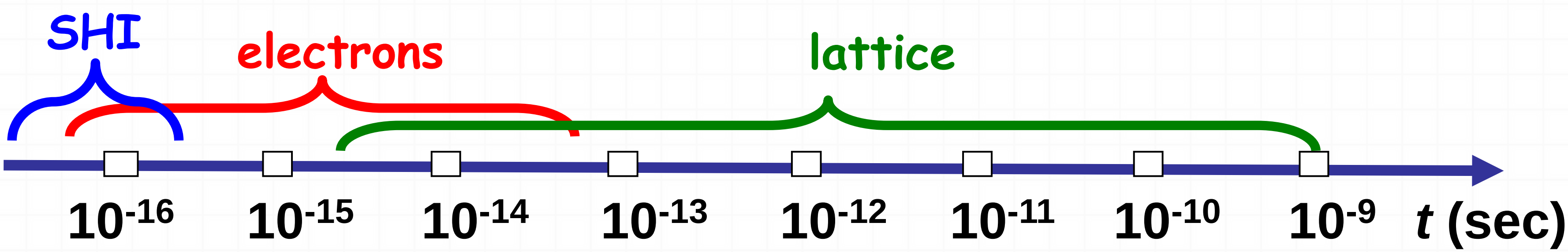


Marek Skupinski
(Uppsala)

Laser spot (1x1 µm)

SHI Track
10nm x
100µm

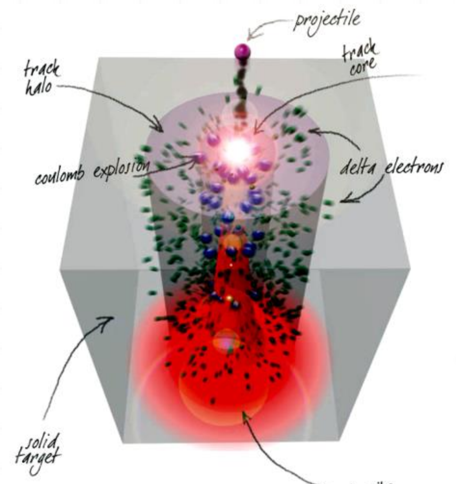




Too fast, too small, too large excitation levels

Can not be described with macroscopic models

SHI track: temporal and spatial scales



Laser spot (1x1 μm)

SHI Track
10nm x
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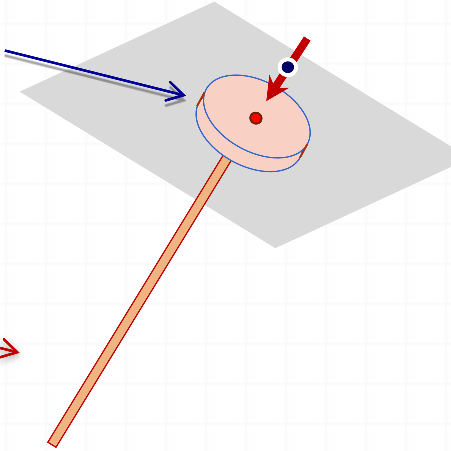
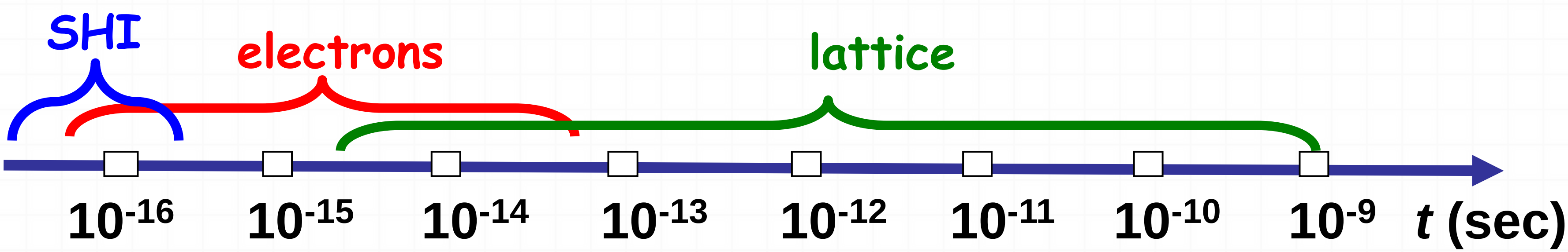
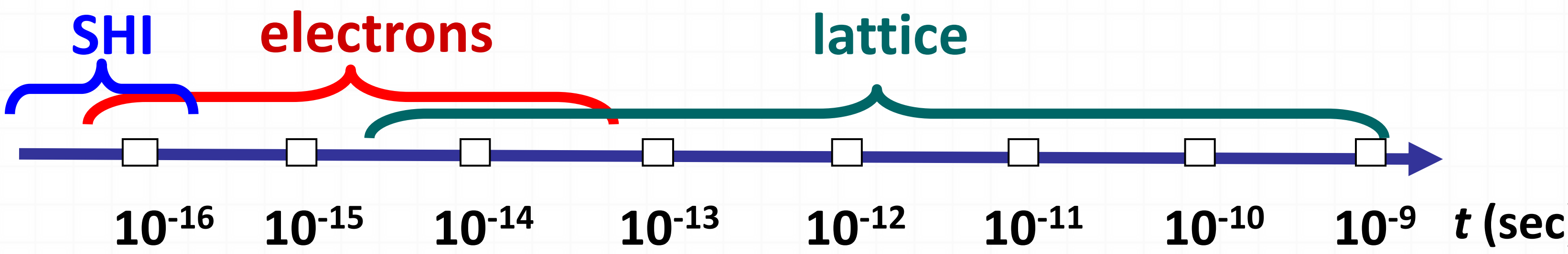




Too fast, too small, too large excitation levels

Can not be described with macroscopic models

Multiscale microscopic model of track excitation



1. Monte Carlo of electronic excitations (10^{-14} s)

Spatial and temporal distributions of holes, fast electrons, their energies and momenta

2. A model of electron-lattice coupling and lattice excitation (10^{-12} s)

Spatial and temporal distributions of energy and momenta transferred into the lattice

3. MD of lattice relaxation (10^{-9} s)

Structure transformations

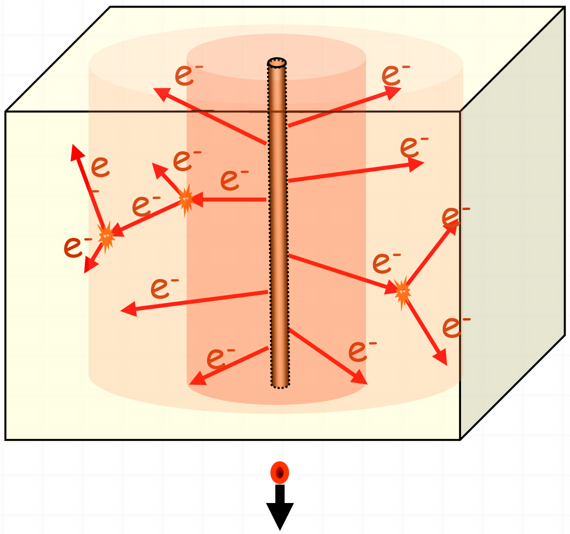
R.A. Rymzhanov et al., J.PhysD .Appl.Phys. 50 (2017) 475301

Monte Carlo (TREKIS) of the initial electronic kinetics

Time-Resolved Electron Kinetics in SHI Irradiated Solids

N.A.Medvedev et *al.*, J. Phys. D Appl. Phys. 48 (2015) 355303

$$t = 10^{-17}\ \mathrm{s} - 10^{-14}\ \mathrm{s}$$



Event by event simulations

Scattering on spatially and dynamically coupled particles

$$\frac{\partial^2\sigma}{\partial\Omega\partial(\hbar\omega)} \sim \left|V(\mathbf{k})\right|^2 \mathrm{Im}\left(\frac{-1}{\varepsilon(k,\omega)}\right)$$

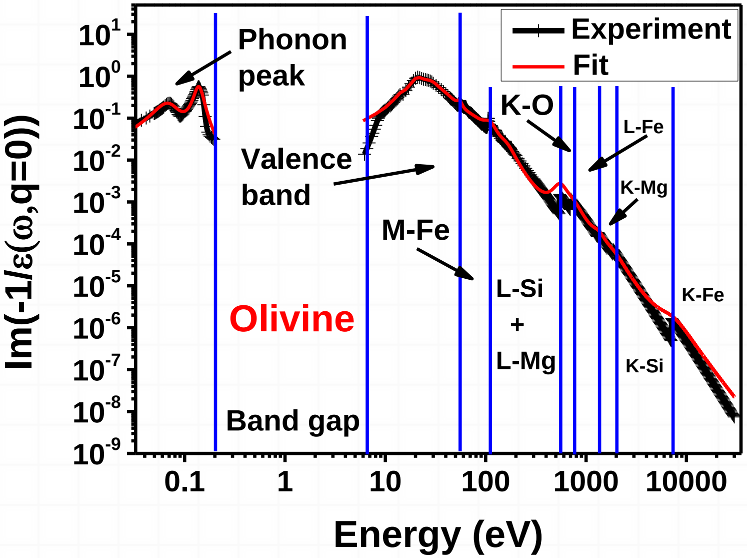
1. **SHI passage and generation of fast primary δ-electrons** **~10^{-17} s**
2. **Spreading of δ-electrons and secondary electron cascading. Creation of secondary electrons and holes** **~10^{-16}-10^{-14} s**
3. **Kinetics of all next generations of electrons and holes** **~10^{-14}s**
4. **Auger decays of deep shell holes ~10^{-15} s**
5. **Radiation decay and photons transport**

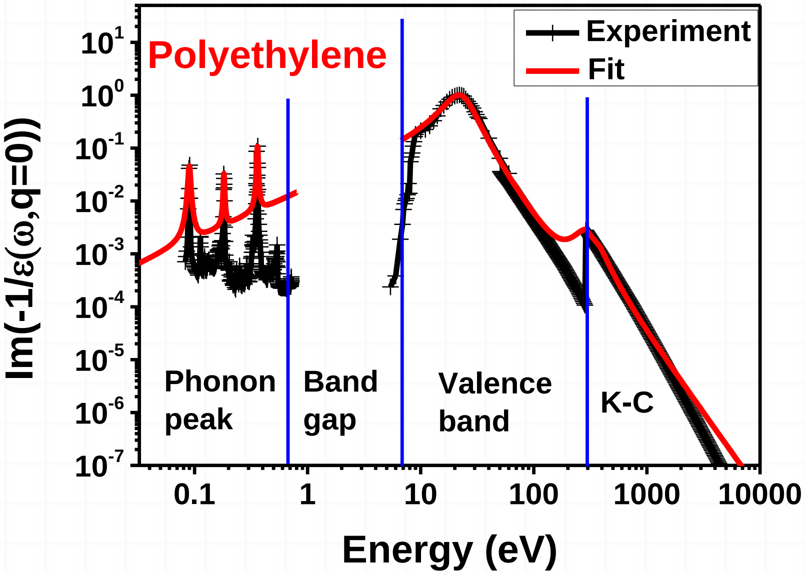
Complex Dielectric Function

e.g. Ritchie and Howie formalism

- individual scattering: ionization of the valence band or deep shells
- collective scattering: plasmons, phonons etc.

$$\frac{\partial^2 \sigma_{el}}{\partial k \partial(\hbar\omega)} \sim \mathrm{Im}\left[\frac{-1}{\varepsilon(\omega,q)}\right] = \sum_{i=1}^{n^{os}} \frac{A_i \gamma_i \hbar\omega}{[\hbar^2\omega^2 - (E_{0i} + \hbar^2 q^2/(2m_e))^2]^2 + (\gamma_i \hbar\omega)^2}$$

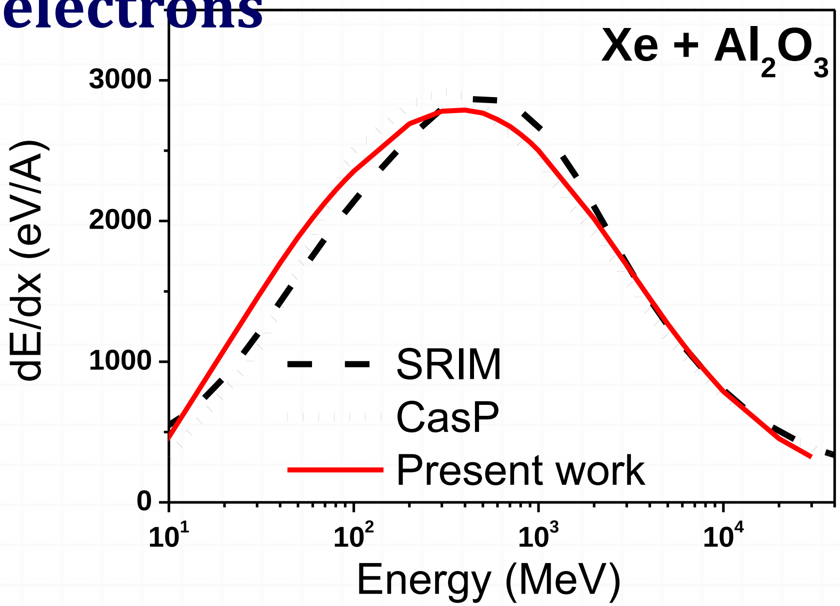


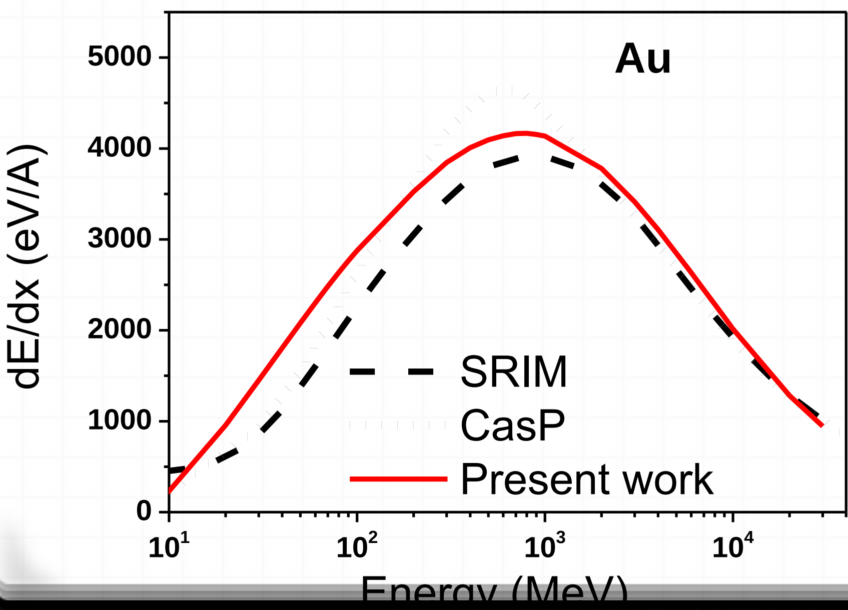


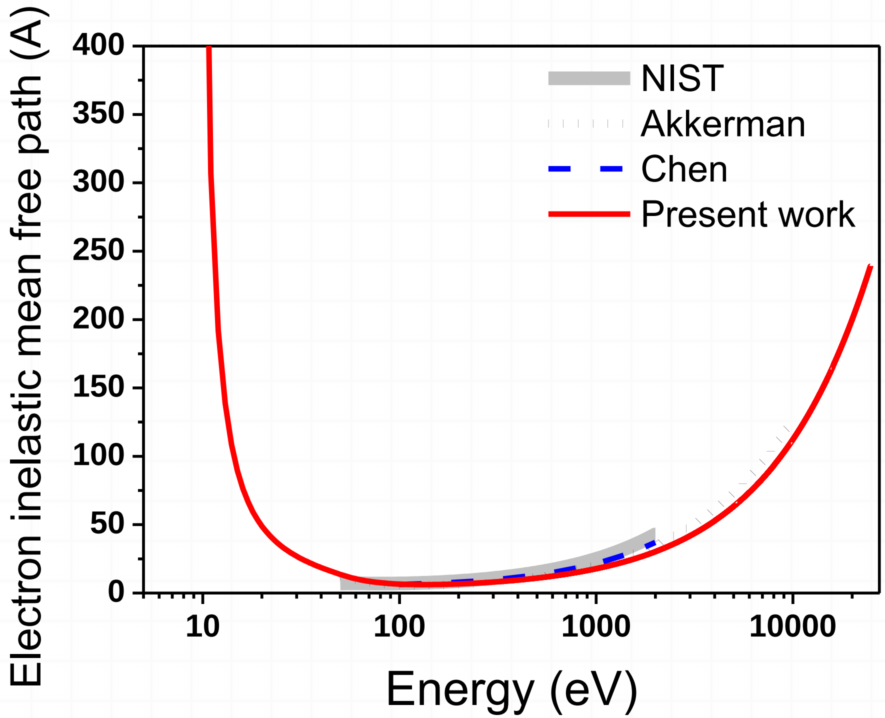
N.A.Medvedev et *al.*, J. Phys. D Appl. Phys. 48 (2015) 355303

TREKIS: Verification of model

Electronic energy loss of ions and inelastic mean free paths of electrons



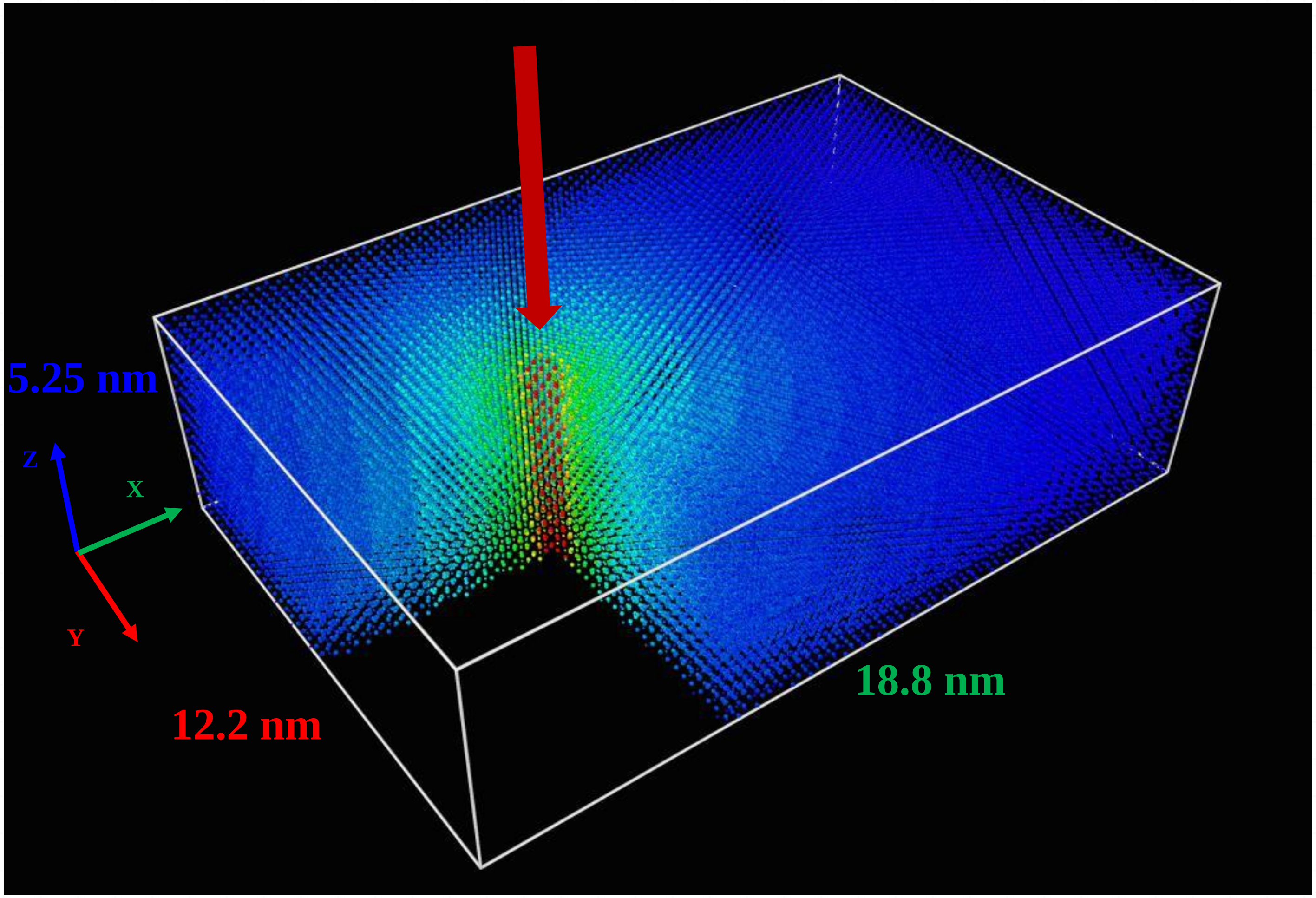




Good coincidence with SRIM, CasP and NIST database

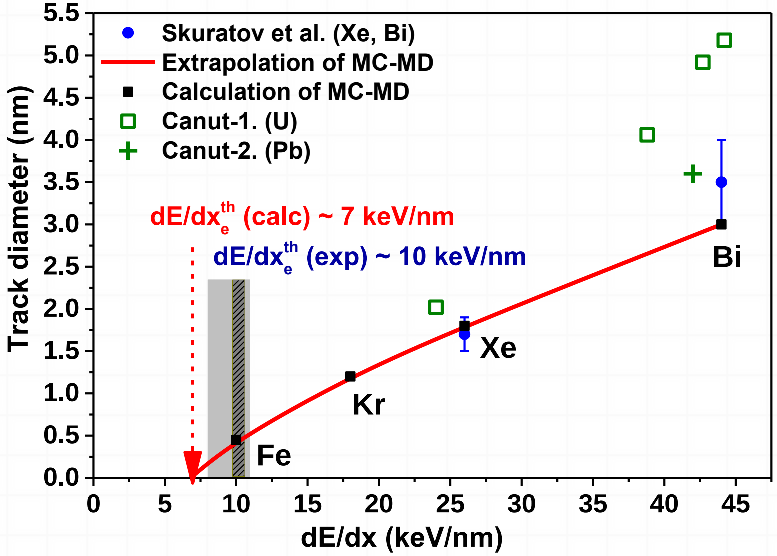
Rymzhanov, Medvedev, Volkov, NIMB 388, 41 (2016)

MC TREKIS + MD LAMMPS



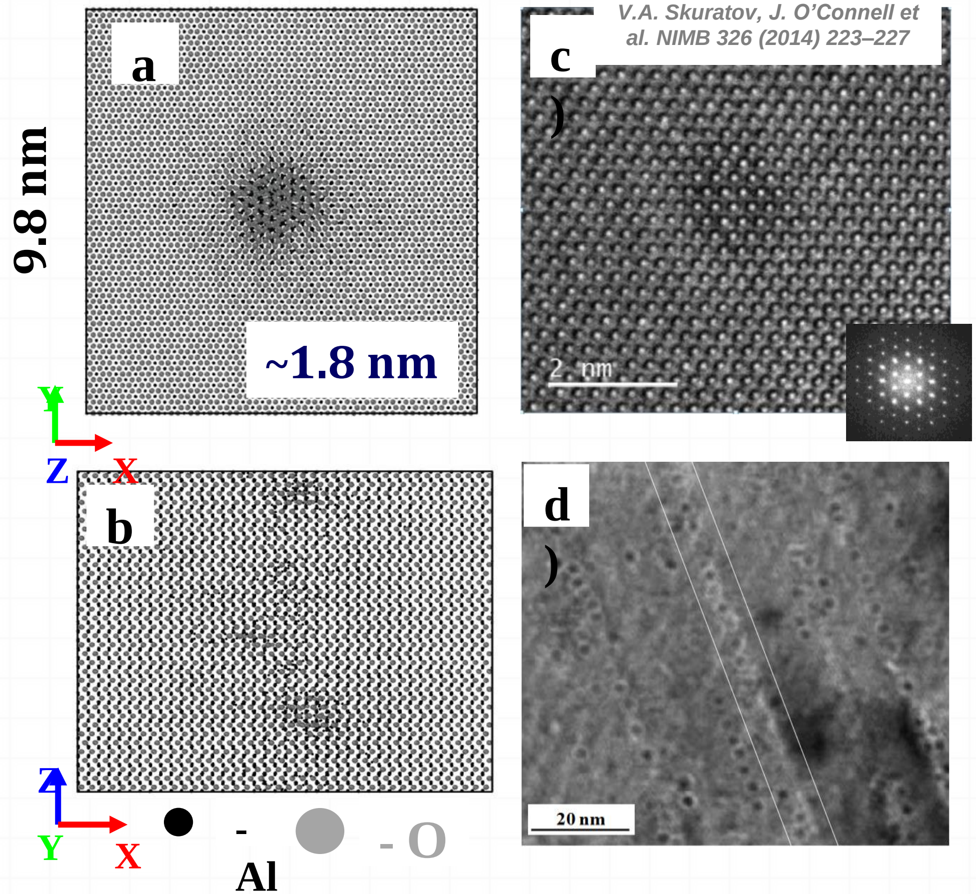
MD code LAMMPS *Plimpton S. J. Comput. Phys. 117 (1995) 1–19*

Threshold and morphology of tracks in Al_2O_3



$(dE/dx)^{th}$ ~ 7 keV/nm

(~ 3.2 ± 0.4 eV/atom)

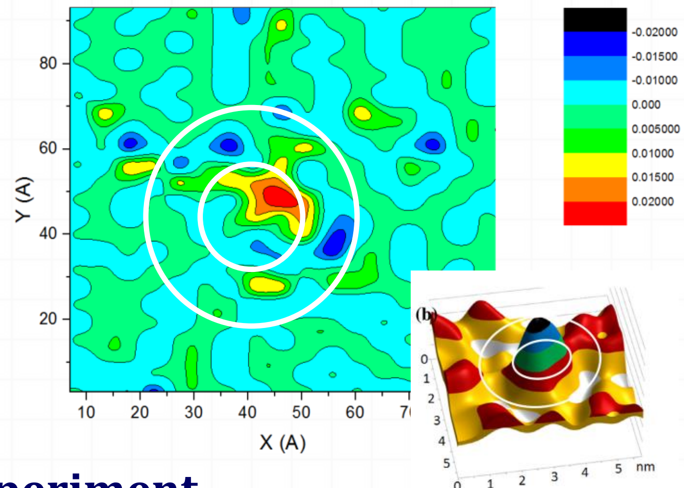


167 Mev Xe
Crystalline damaged discontinuous track of 1.8 nm diameter after 50 fs

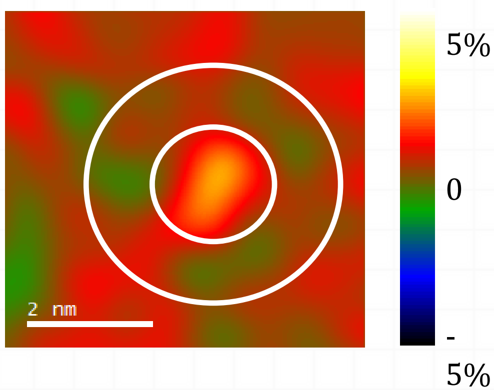
Residual strain of Xe 167 MeV track in Al_2O_3

Lattice deformation:

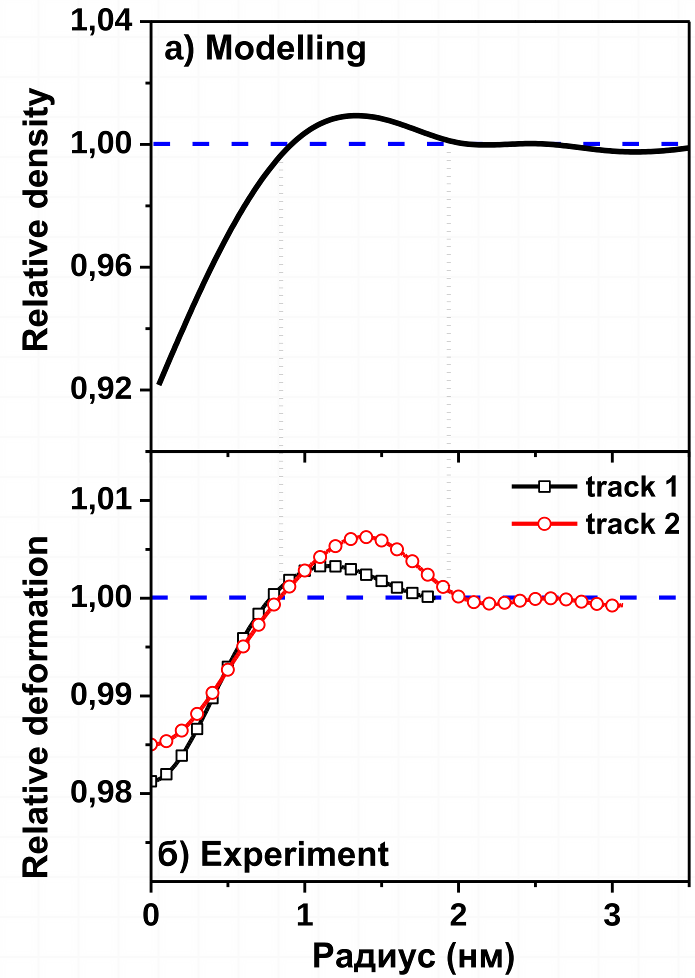
Simulations



Experiment



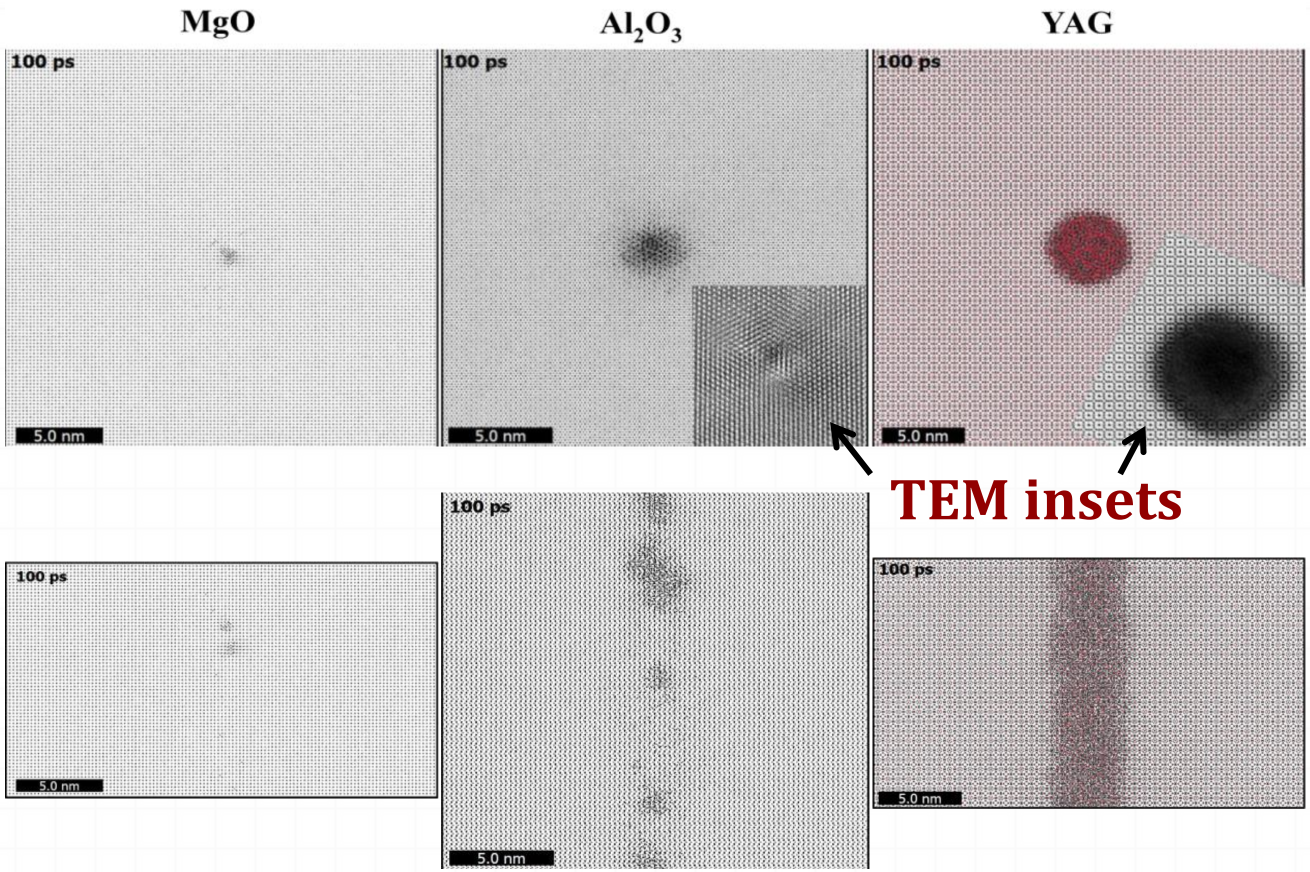
Radial density of Al_2O_3



underdense core is surrounded by overdense shell

O'Connell et al., NIMB 374 (2015) 97

Recrystallization of tracks in different dielectrics



MgO - only point defects were created

Al_2O_3 - crystalline discontinuous track of D ~ 2 nm

YAG - continuous amorphous track of D ~ 6.5 nm

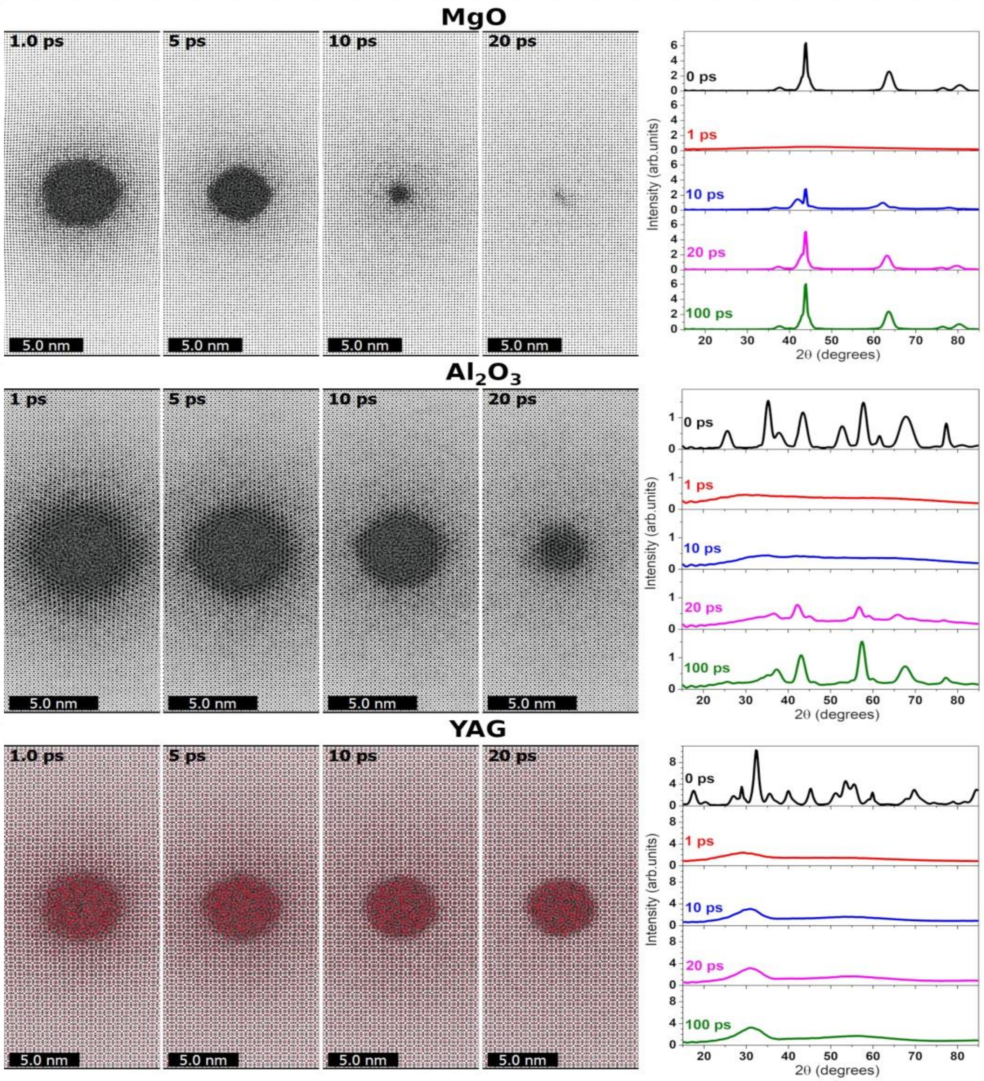
R.A. Rymzhanov et al., Scientific Reports 9 (2019) 3837

Recrystallization plays a crucial role for track formation in MgO, Al_2O_3 and YAG

MgO

Al_2O_3

YAG



nearly perfect recrystallization

partial recovery

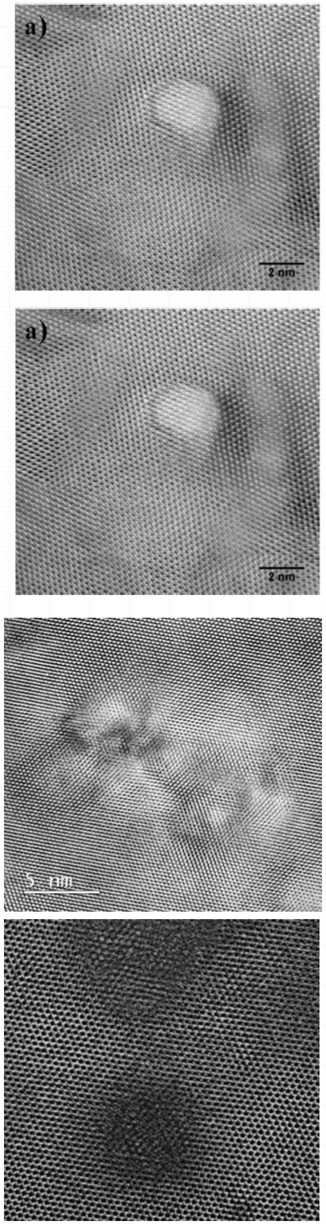
almost no recovery

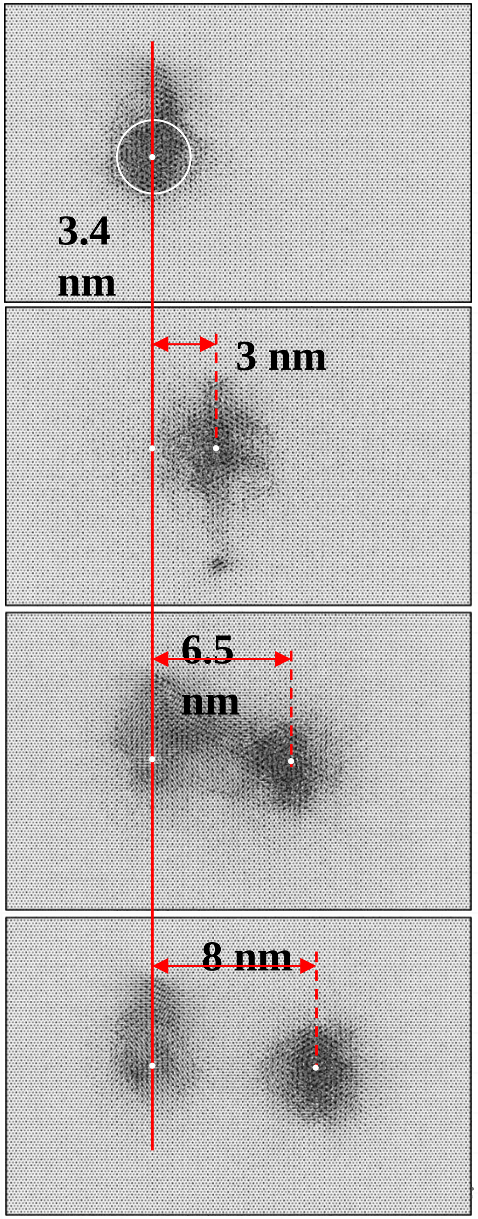
R.A. Rymzhanov et al., Scientific Reports 9 (2019) 3837

Overlapping of SHI tracks.

Bi 700 MeV in Al_2O_3

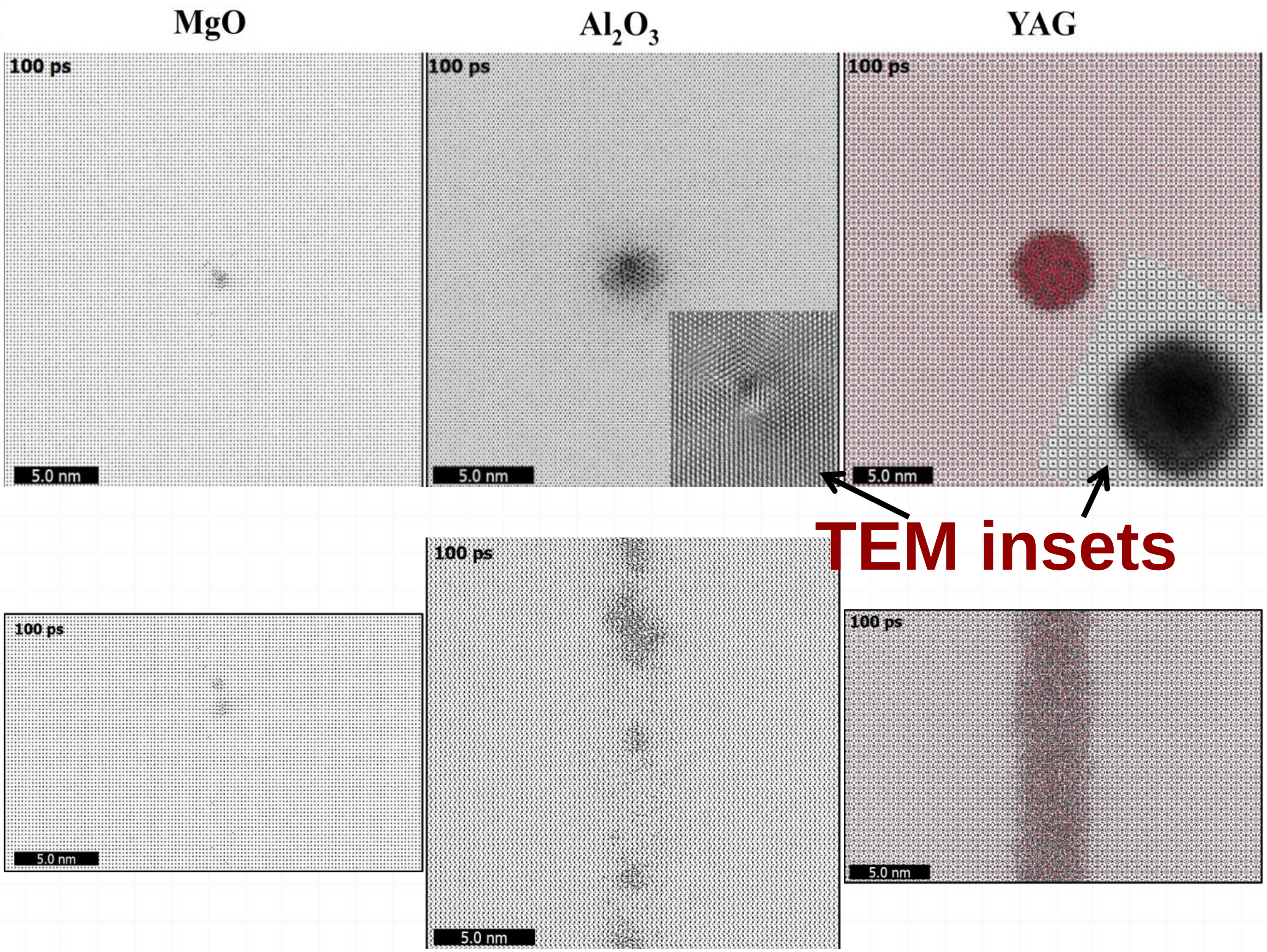
- **Second ion causes annealing of defects created by the first one**
- **Ions at longer distances cause partial annealing of older tracks**
- **Radius of recovery is ~ 6.5 nm (experimental ~ 5.4 nm) corresponding to the track density of ~ 2.7×10^{12} cм$^{-2}$**





R.A. Rymzhanov, et.al, NIMB 435 (2018), 121-125

Recrystallization during track formation propcess



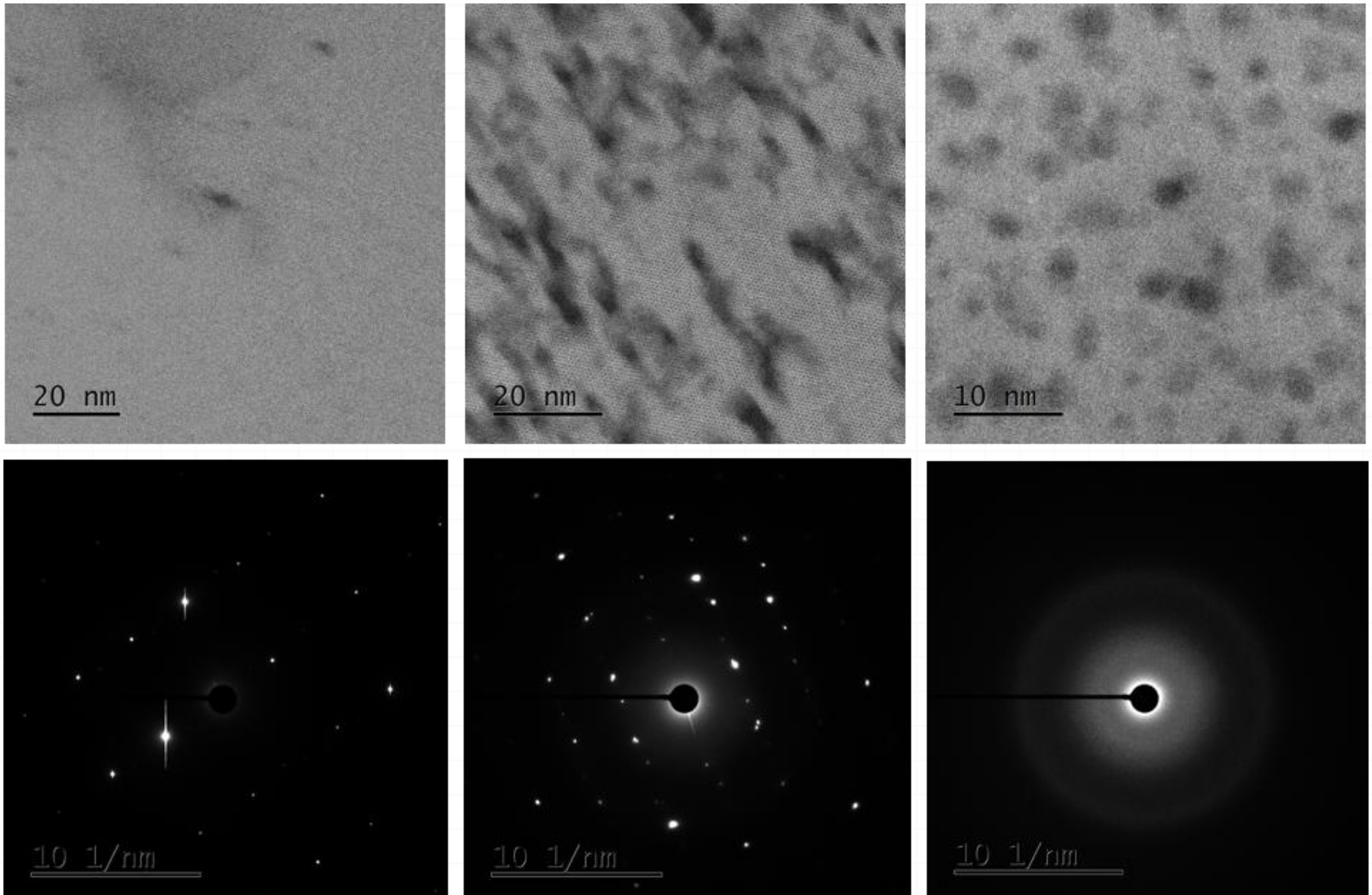
MgO - only point defects were created around the ion trajectory

Al_2O_3 - crystalline discontinuous track with the diameter about 2 nm

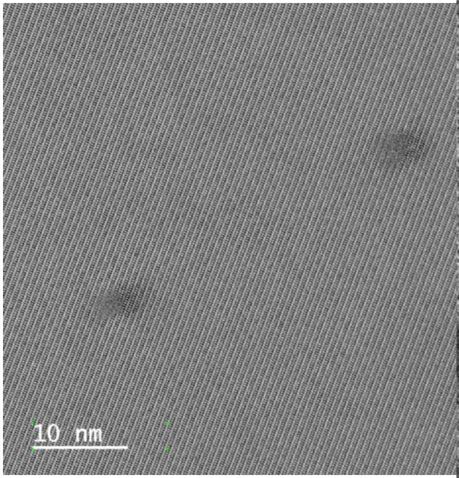
YAG - continuous amorphous track of ~6.5 nm in diameter

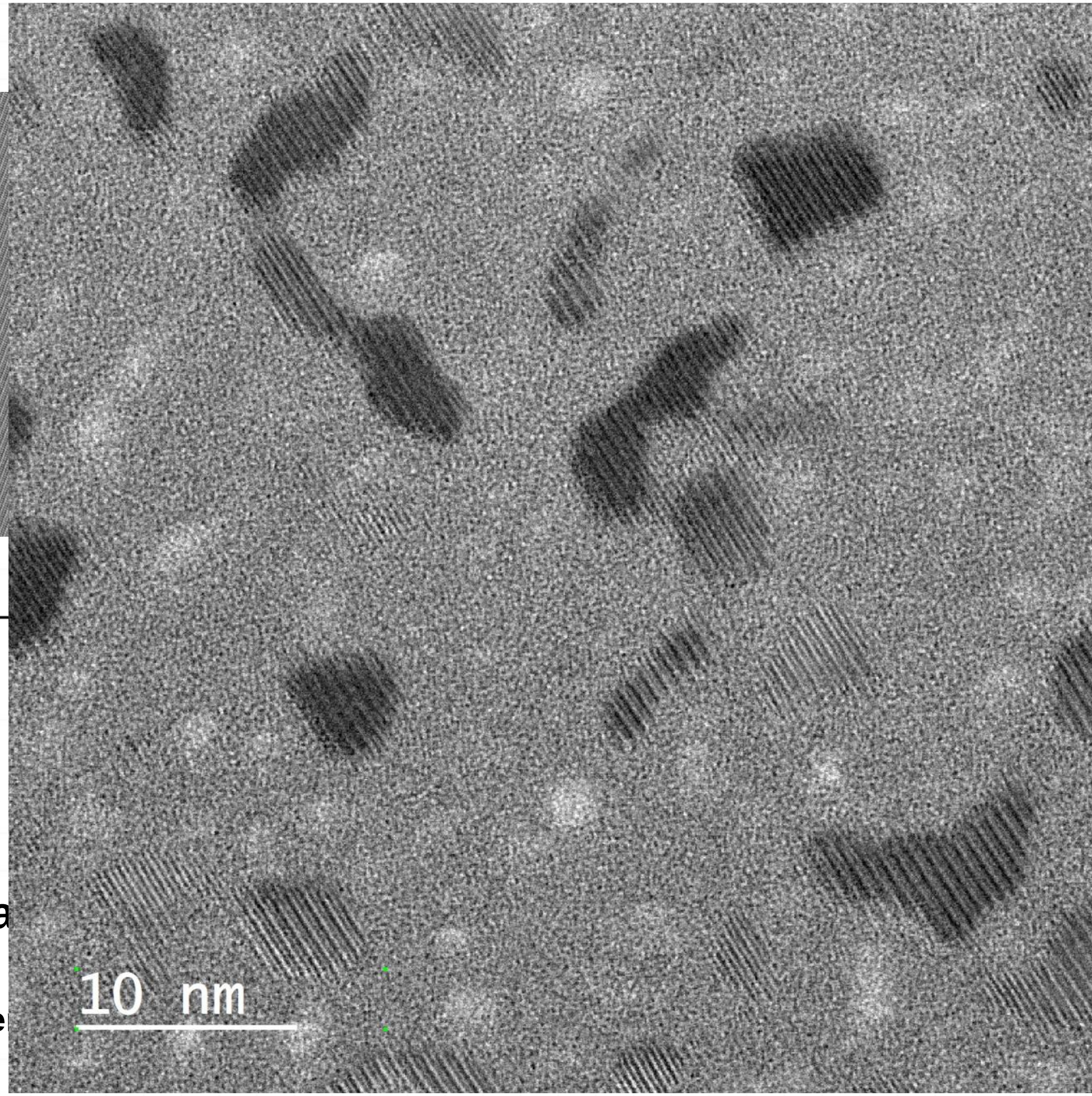
p-Si_3N_4 + Xe 220 МэВ

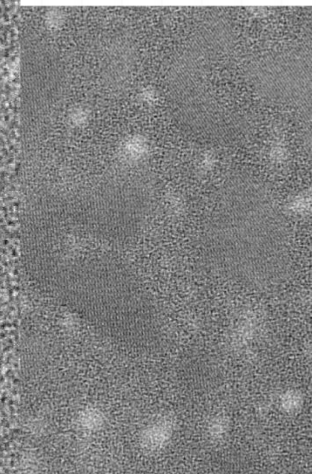
$5x10^{11}$ см$^{-2}$ | $1x10^{13}$ см$^{-2}$ | $2x10^{14}$ см$^{-2}$

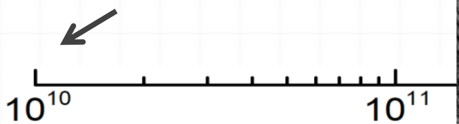


Si3N4 +Bi, 700 MeV







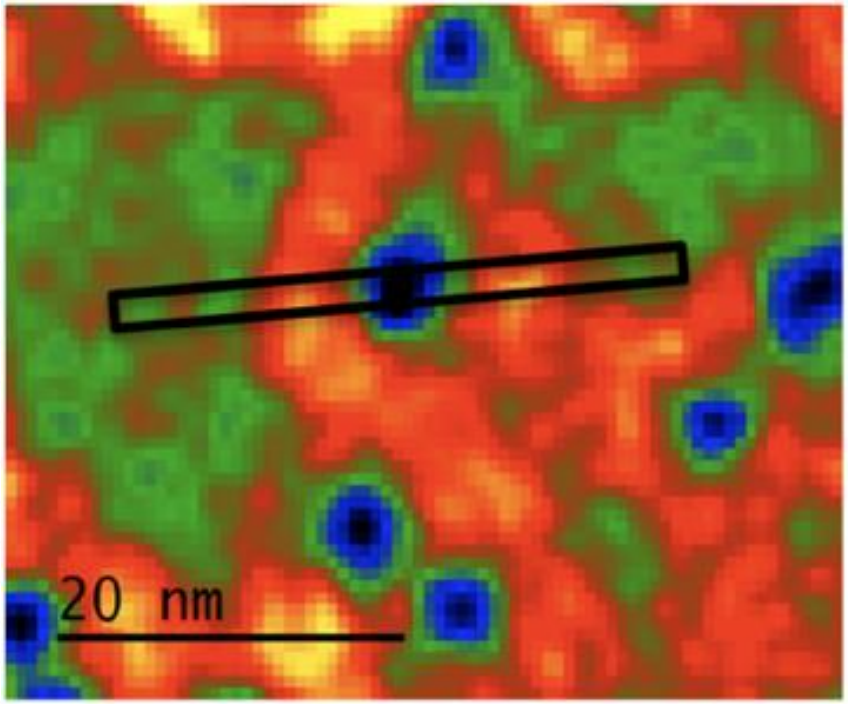


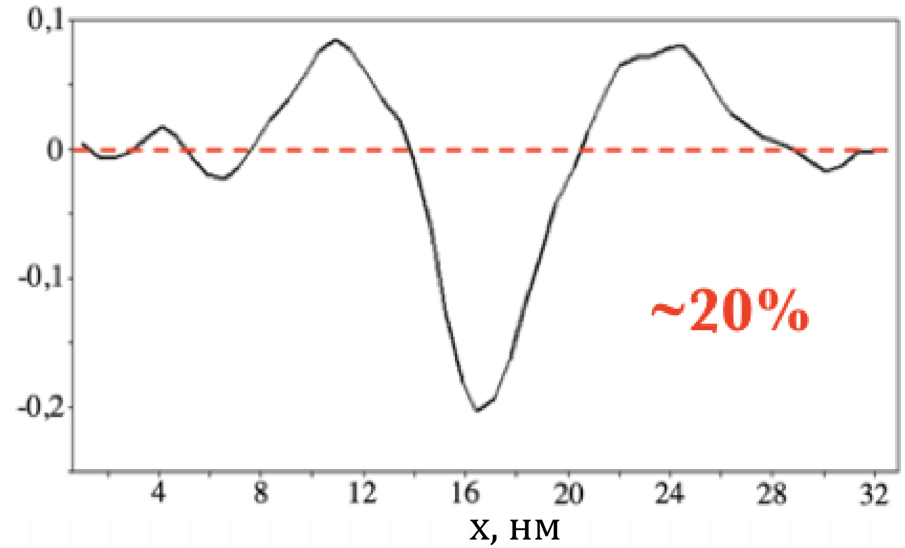
Amorphous tracks

Ion fluence for la

R=1.65 nm Φ_{ove}

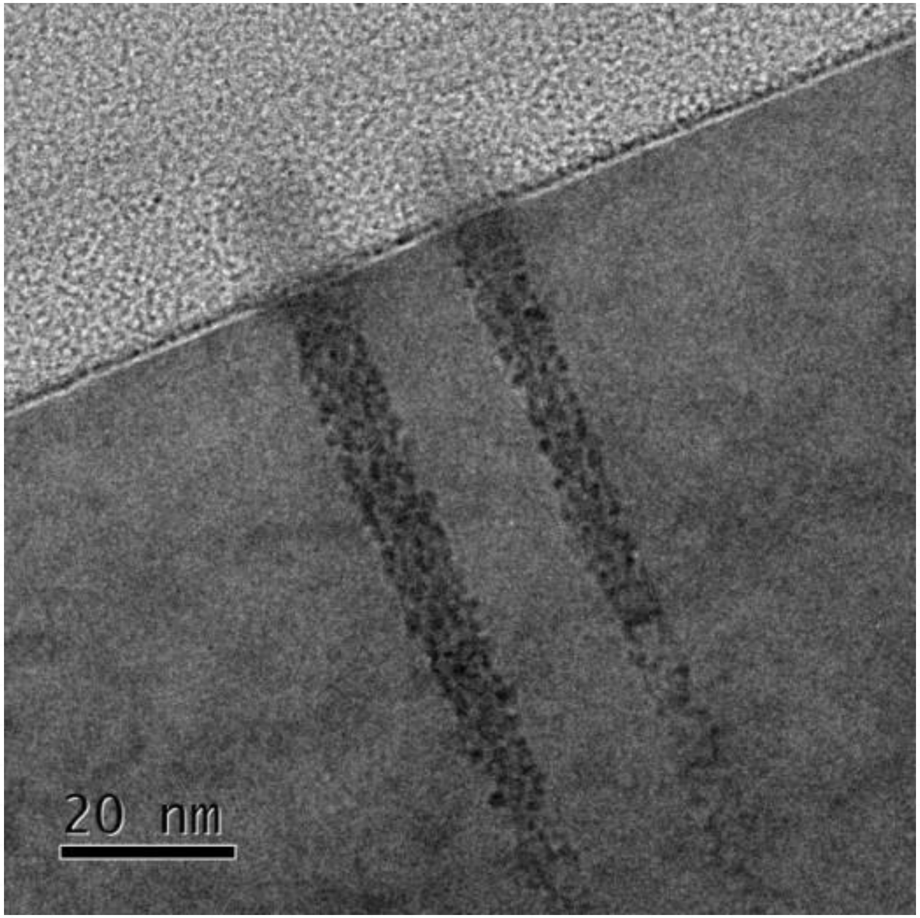
a-Si_3N_4 + Bi 710 МэВ, $5x10^{10}$ см$^{-2}$

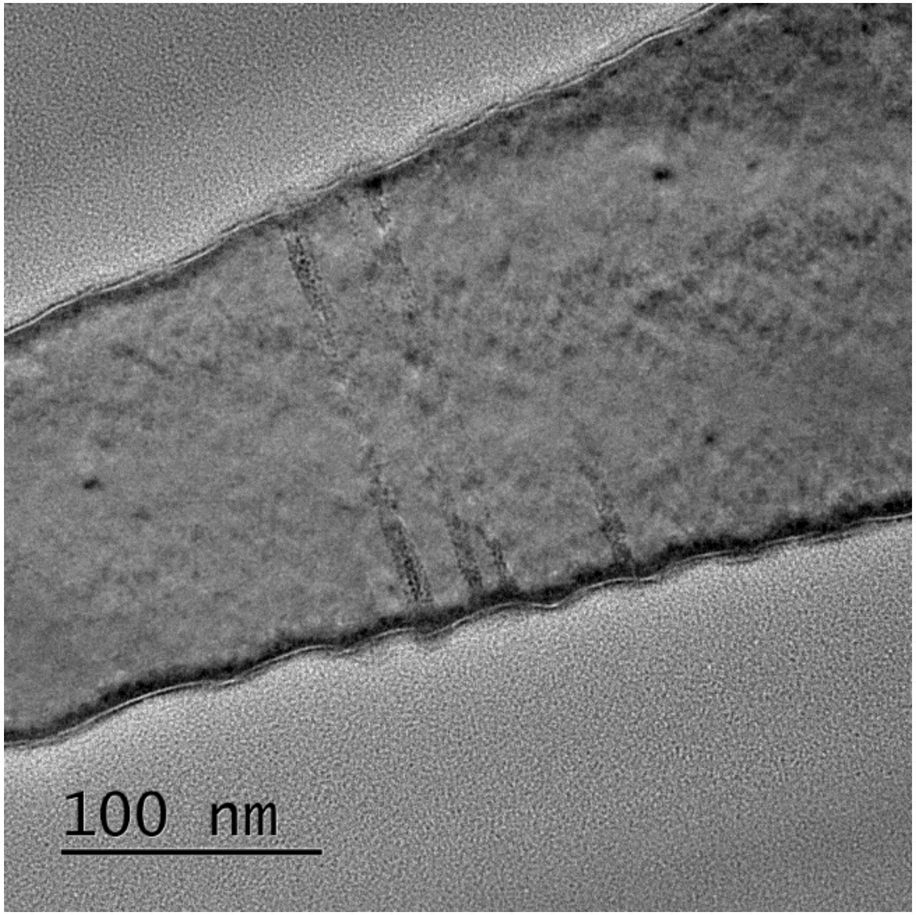




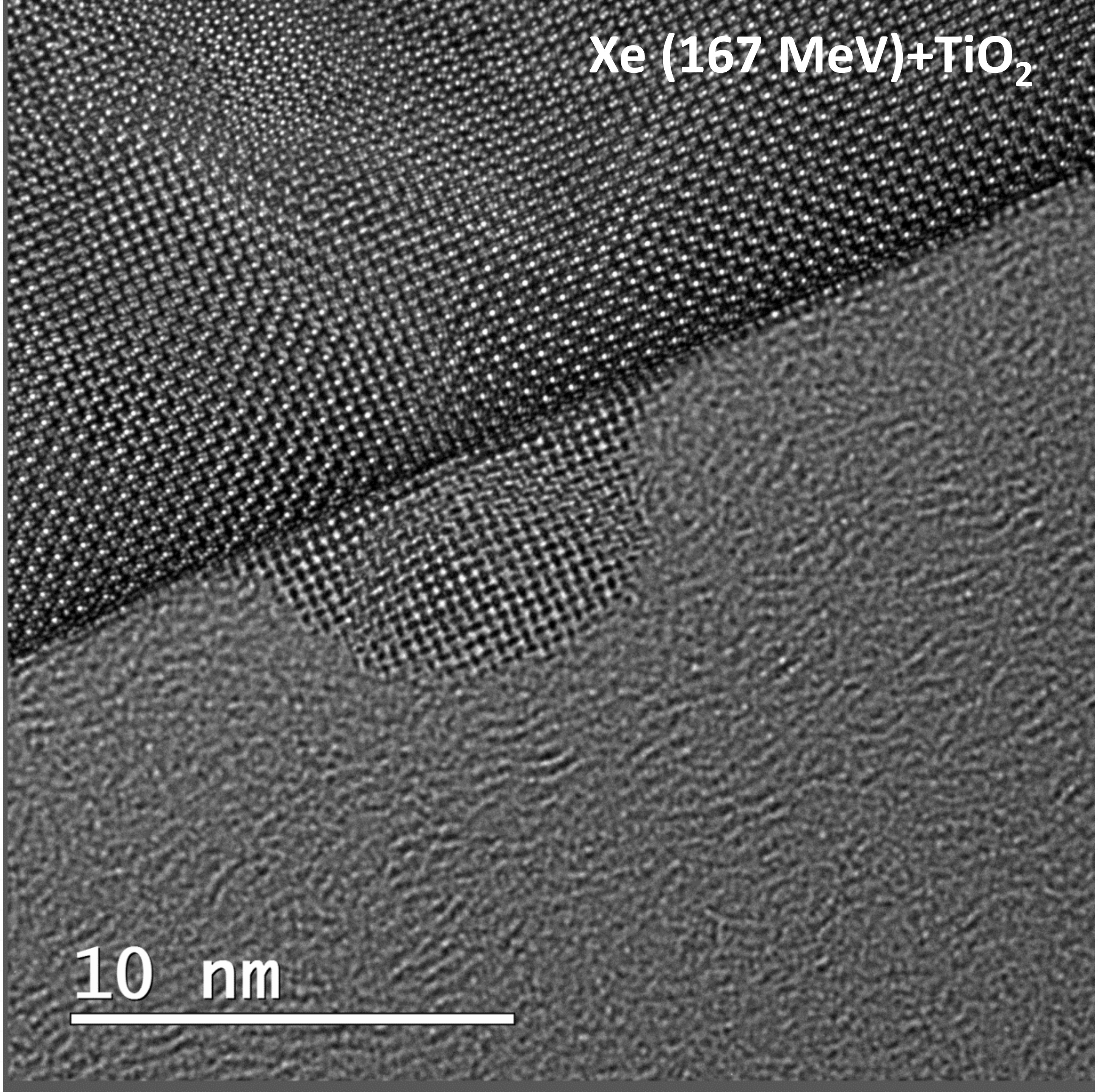
Radial density of Si_3N_4

Surface effects of dense ionization in ceramics and oxides

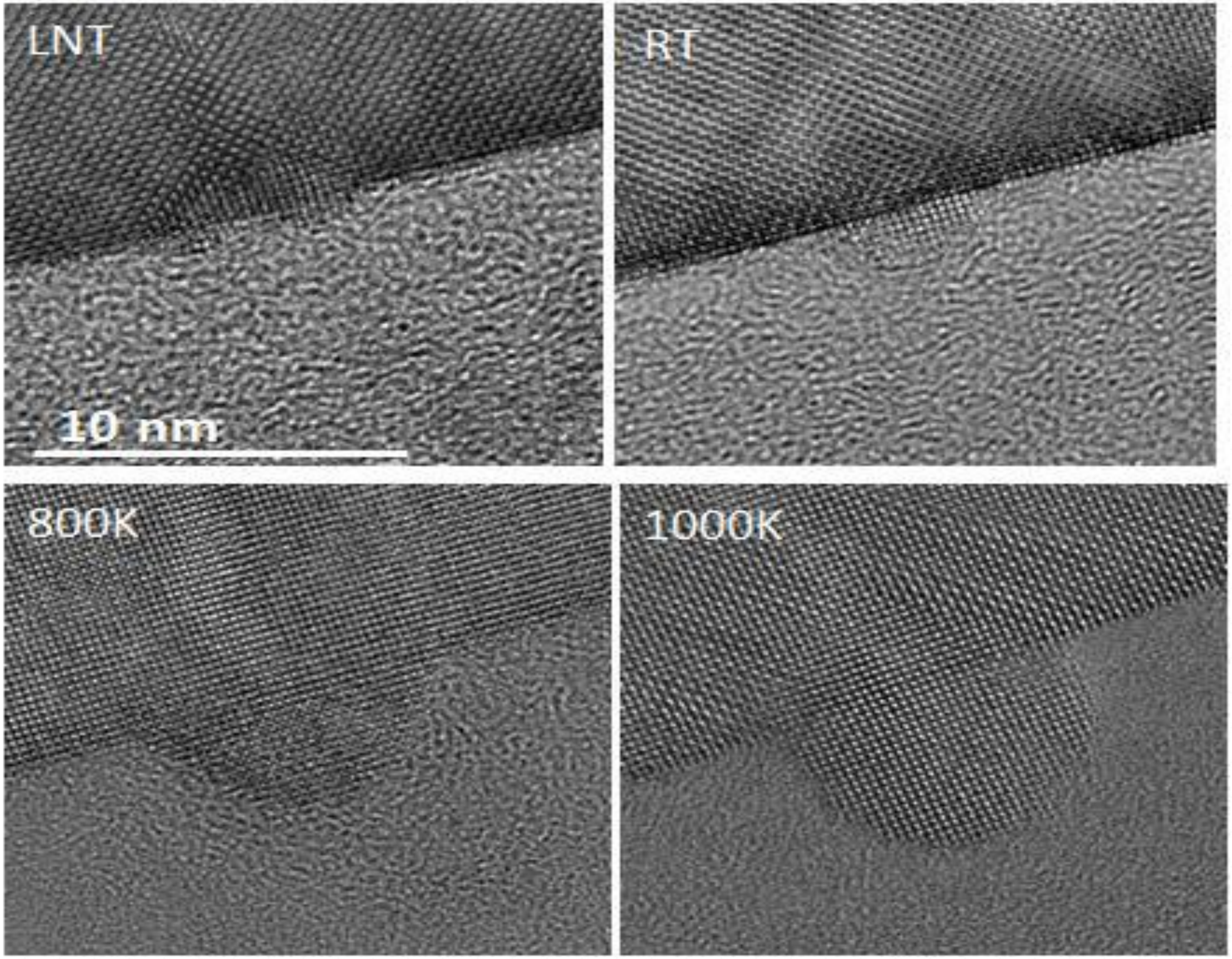




167 MeV Xenon ion induced hillocks in TiO_2


Xe (167 MeV)+TiO_2
10 nm

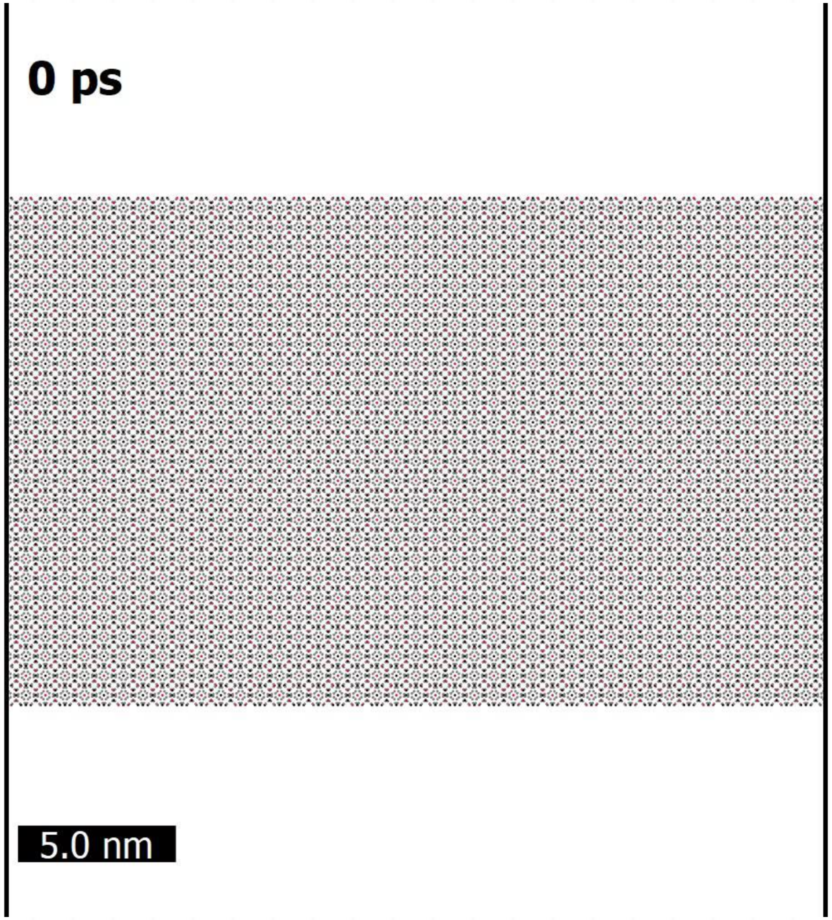
Surface effects of dense ionization in ceramics and oxides

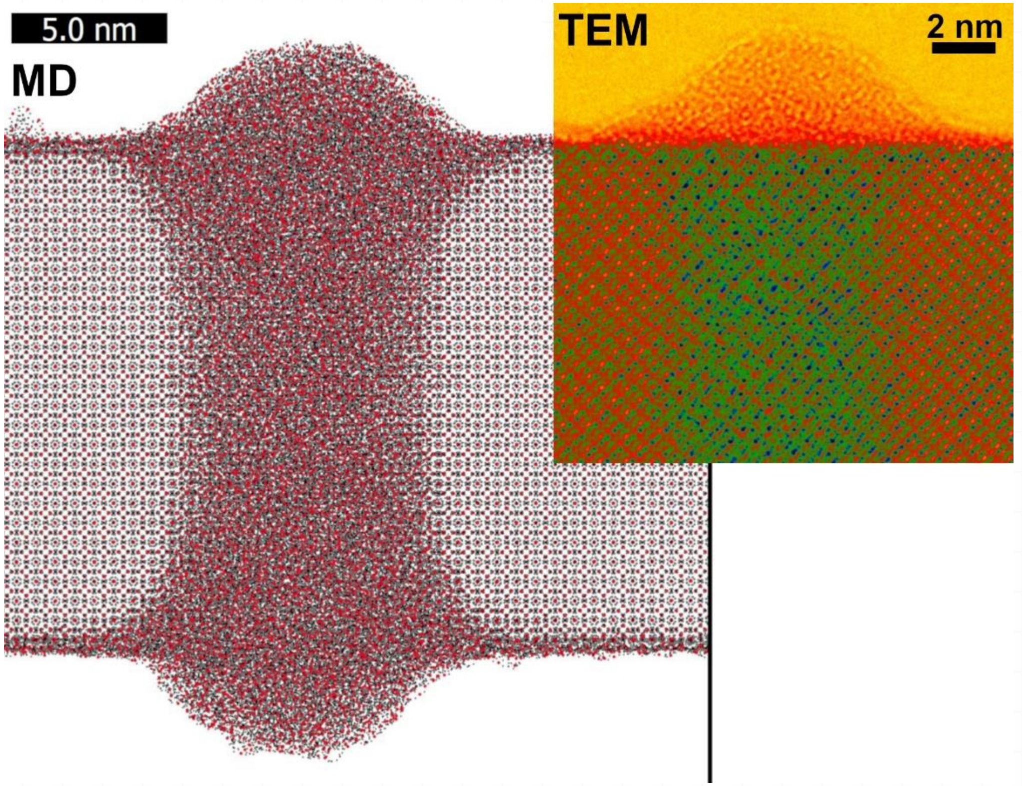


Xe (220 MeV) + TiO_2: Hillock size vs irradiation temperature

Amorphous hillocks in YAG

Bi 700 MeV ion





YAG demonstrates almost no damage recovery:
amorphous cylindrical track and amorphous hillock

R.A. Rymzhanov et al., J.App.Phys. 2020, 127(1) 015901

Thank you for your attention!