A molecular dynamics study of swift heavy ion irradiation of amorphous silica: the role of thermal effects

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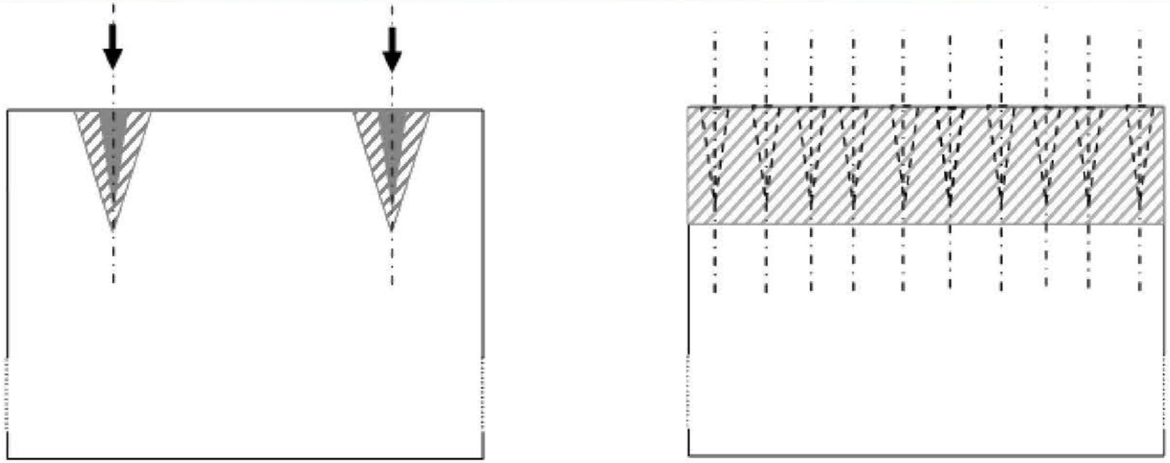
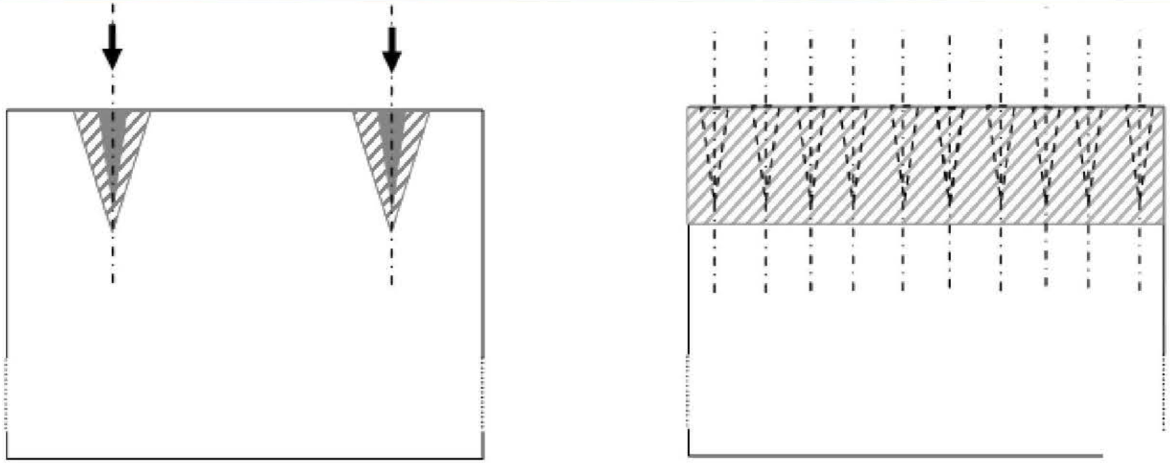
Amorphous silica



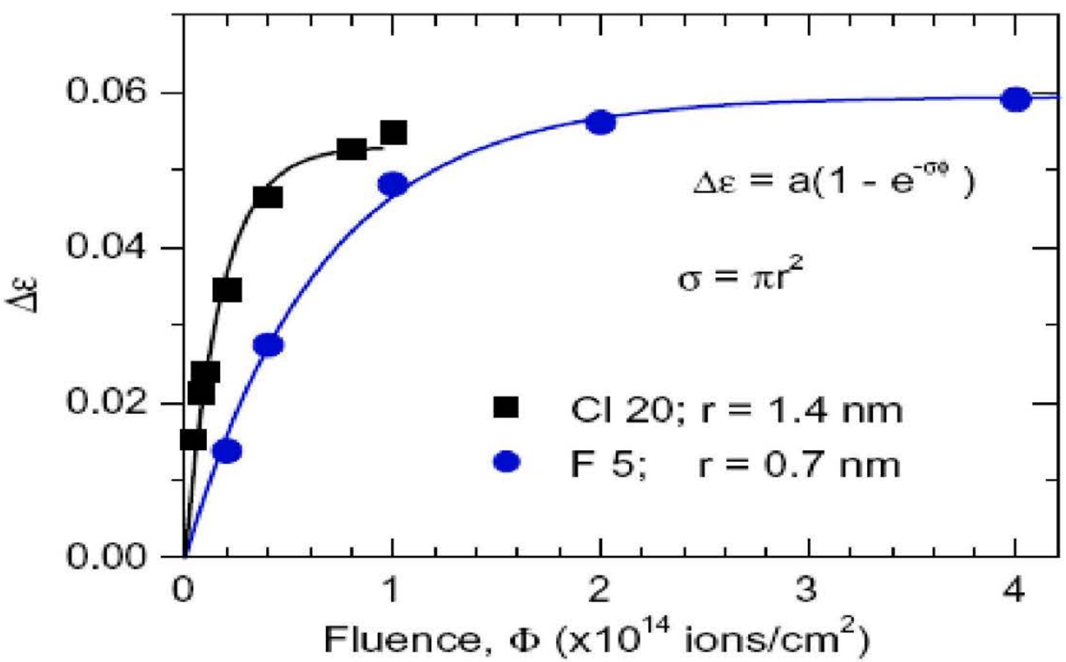
(a) (b)

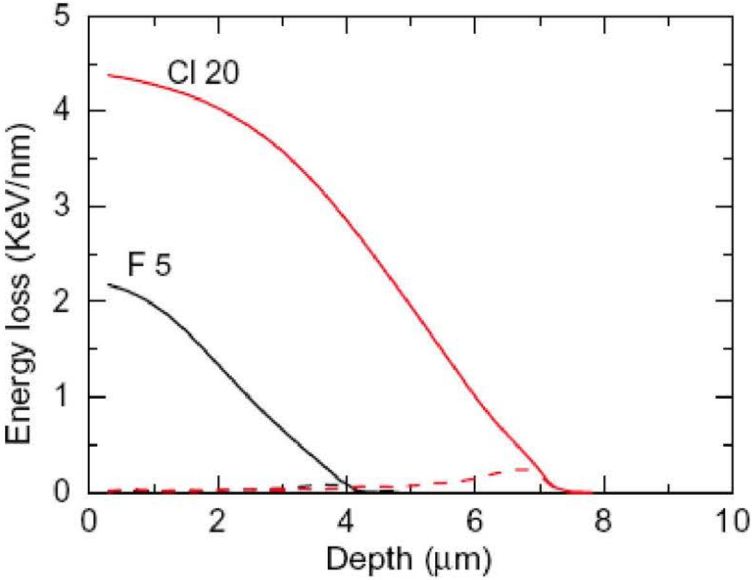
- Swift ion irradiation =>
  - Electronic sputtering
  - Density variation
  - Defect production
- Relevant effects in nuclear fusion

Amorphous silica



- Refractive index change
- Waveguides





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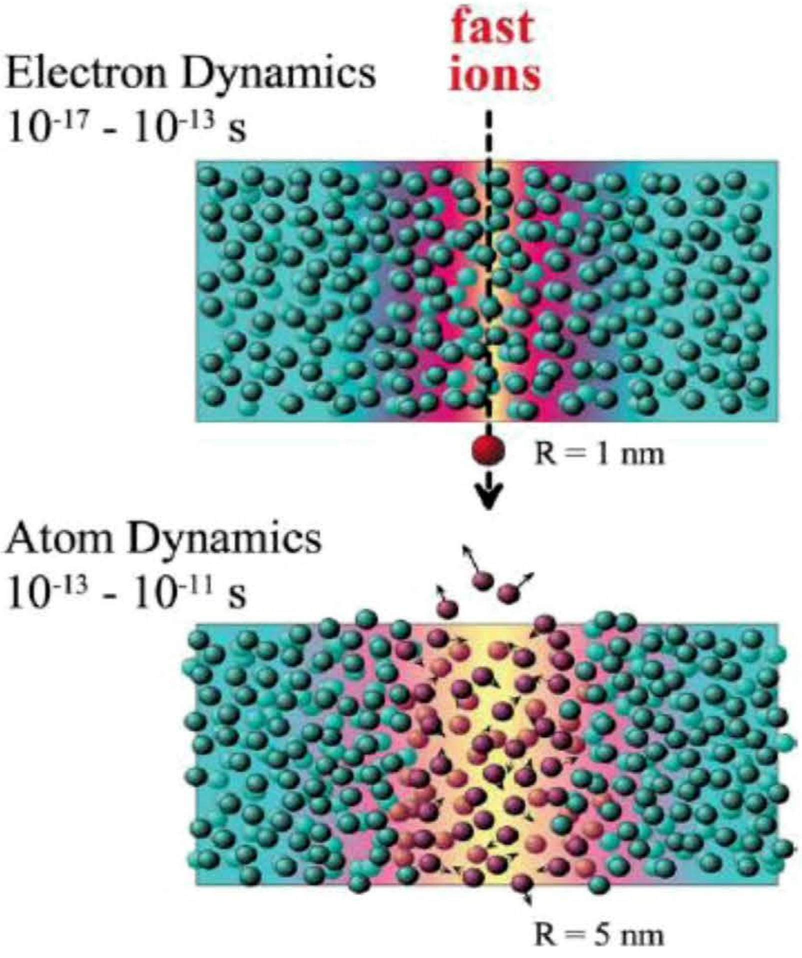
Electronic excitation

- Not well understood
- Permanent damage
- Modification of properties
- Defect annealing
- Nano-track formation
- Complex energy transfer mechanisms

- Goal: thermal effects by MD



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- Super computer MAGERIT CESVIMA UPM
- Typical 512
- Code MDCA
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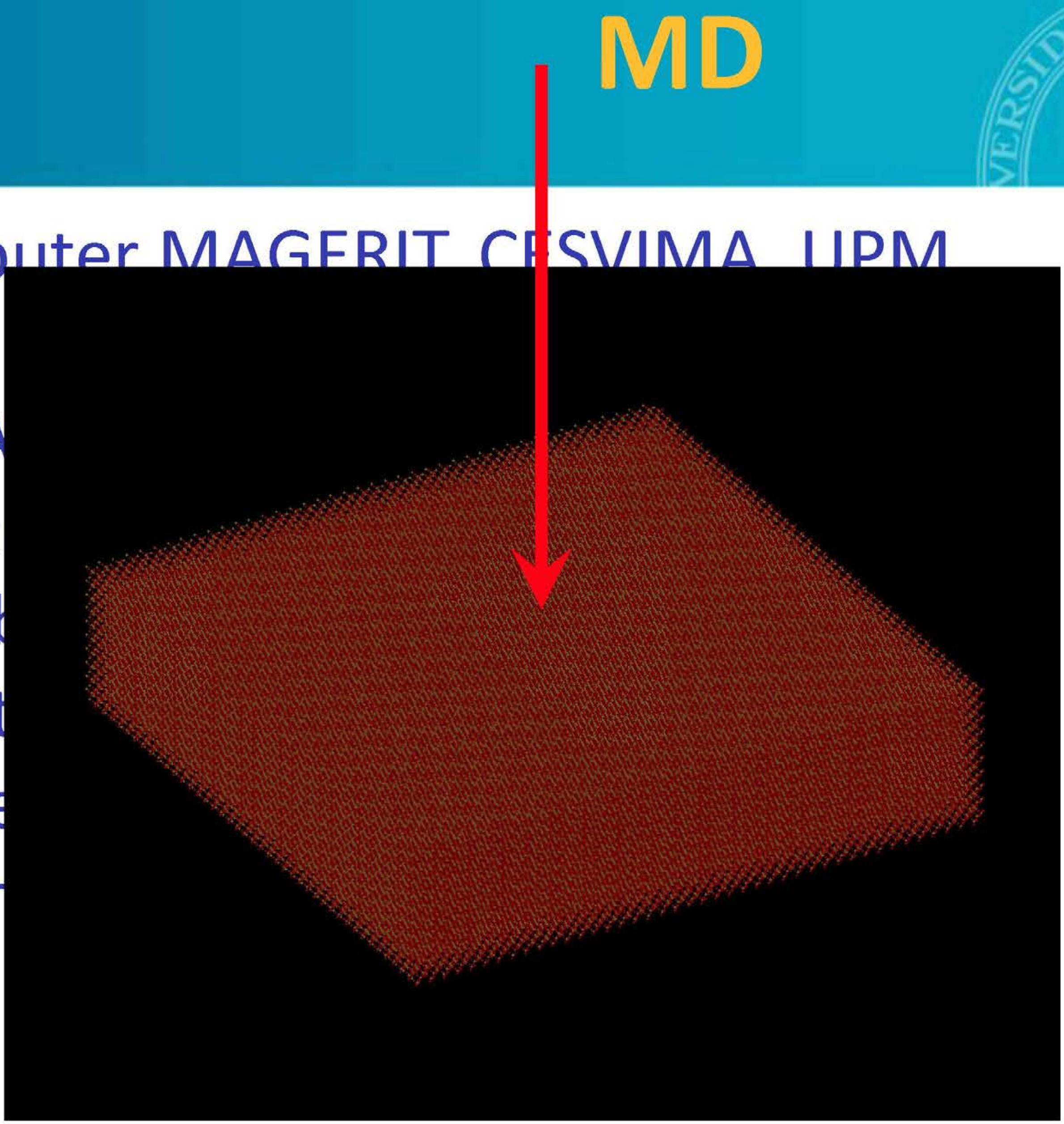

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MD

- Can't explain ion-solid energy transfer
- Our goal is to study thermal effects
- We … power
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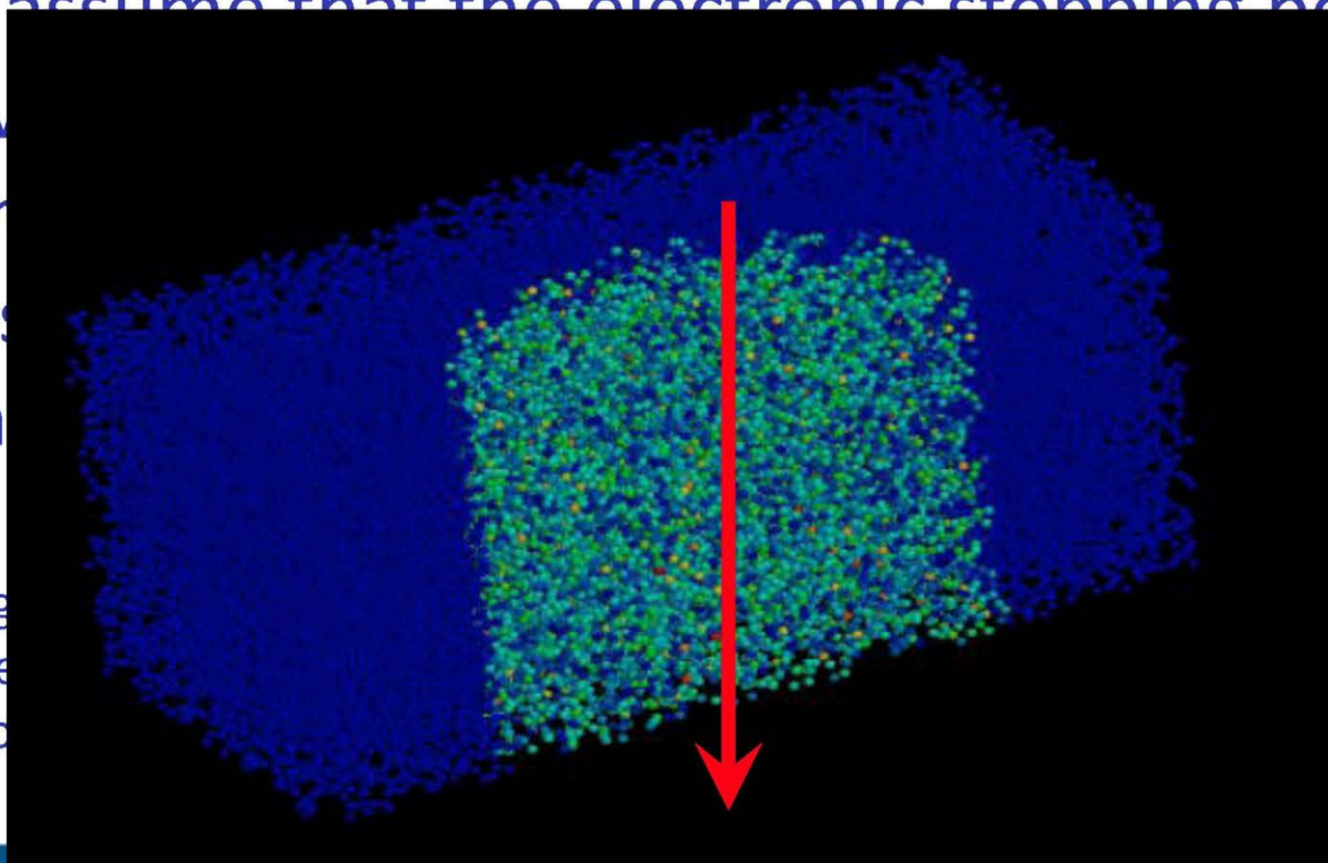
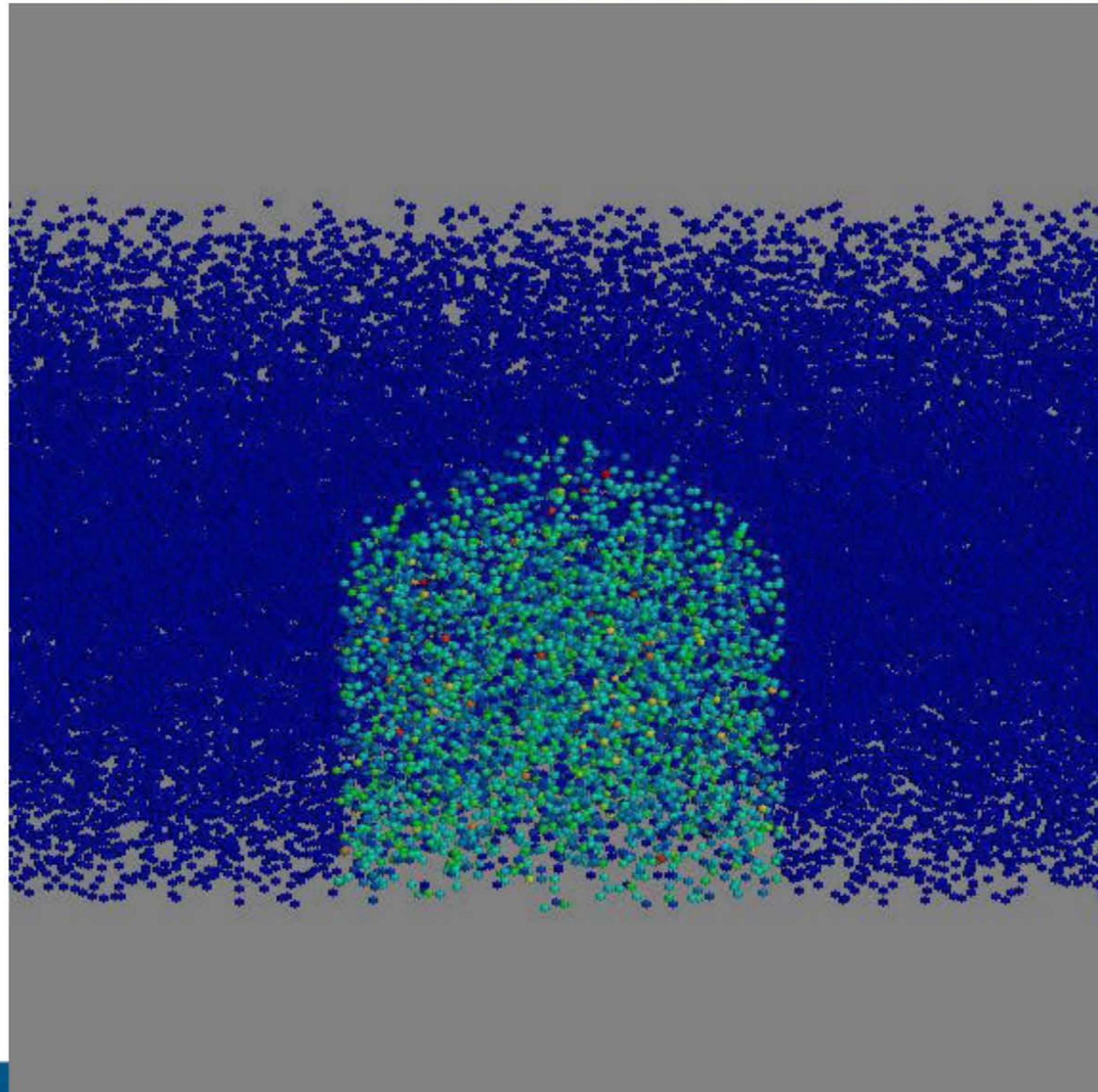


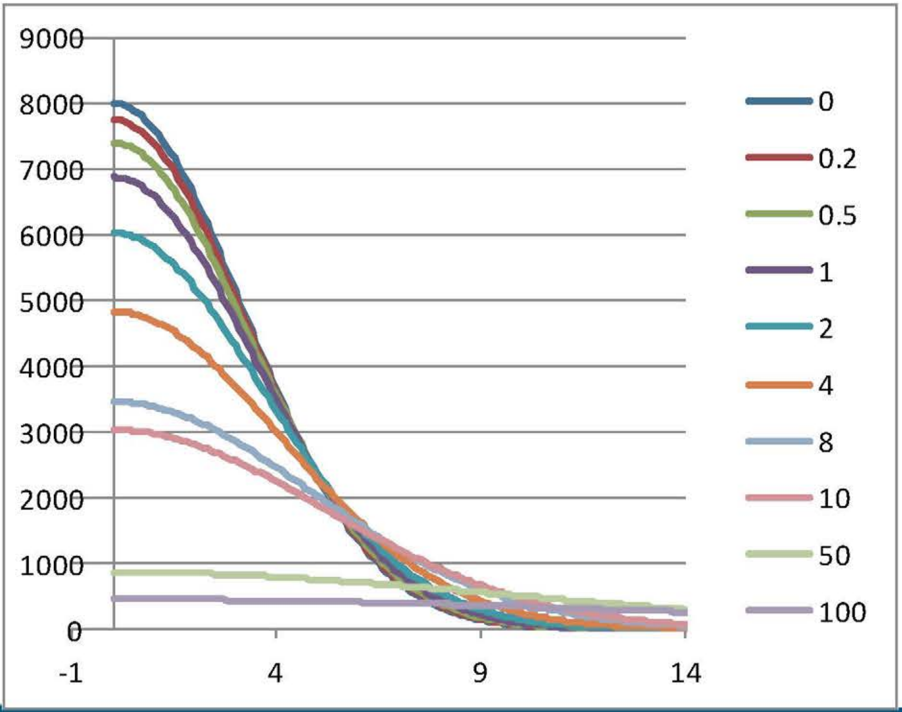
MD

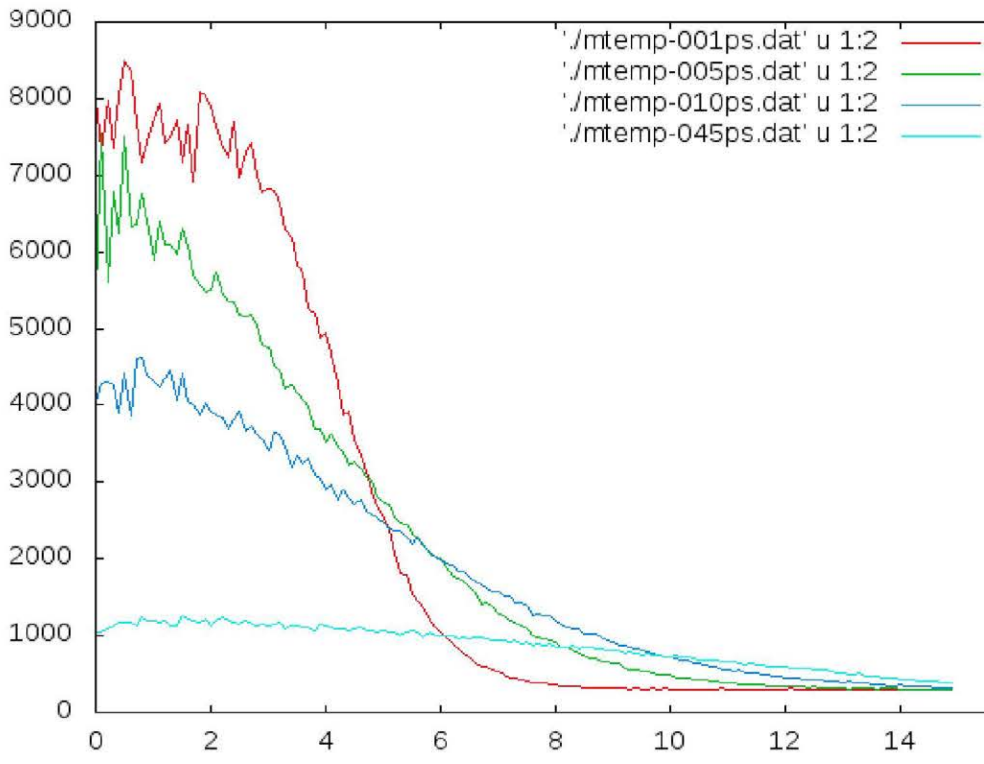


MD

- Resulting temperature profiles compatible with electron MC simulations

10 keV/nm

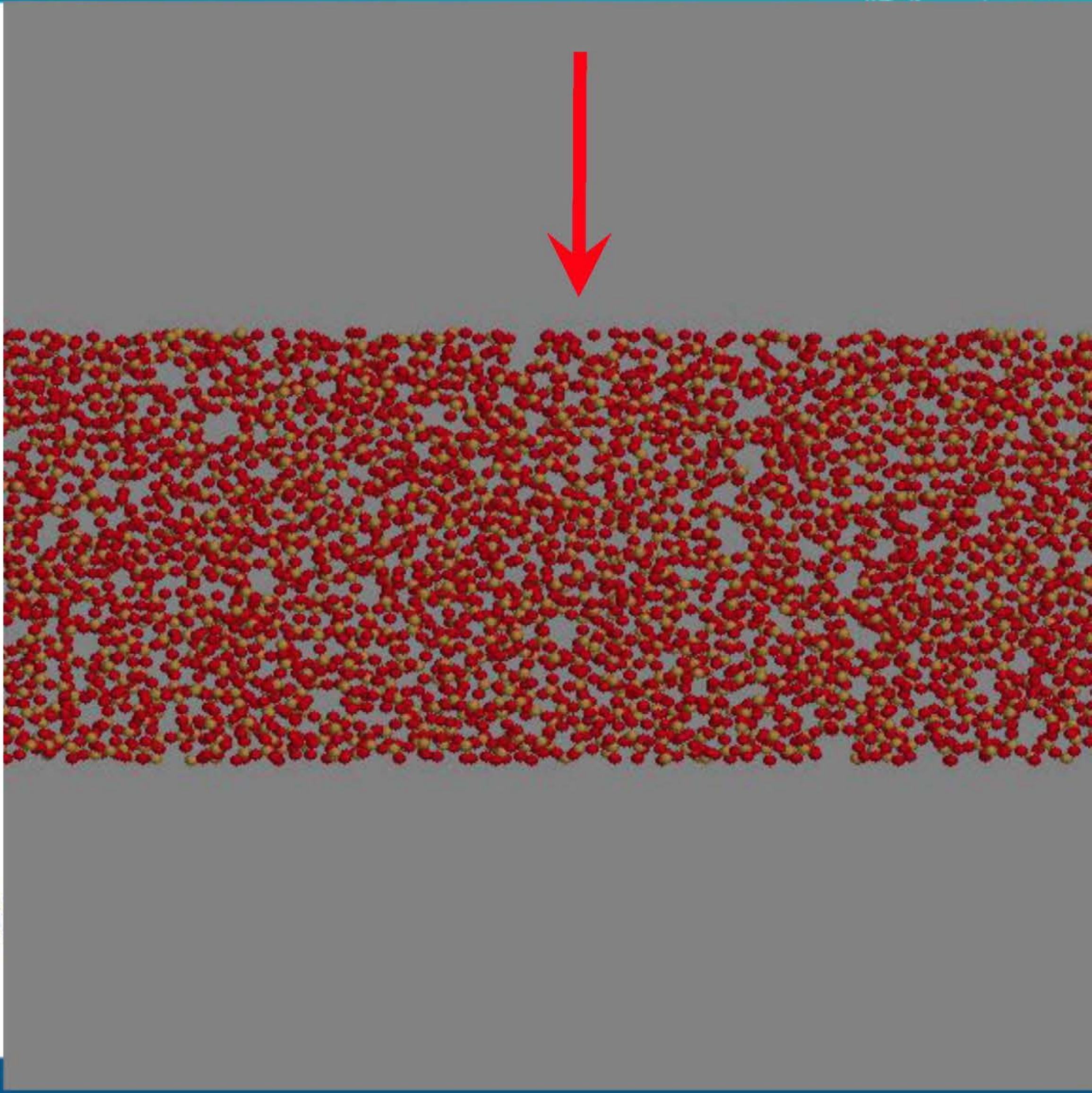




MD

12 keV/nm

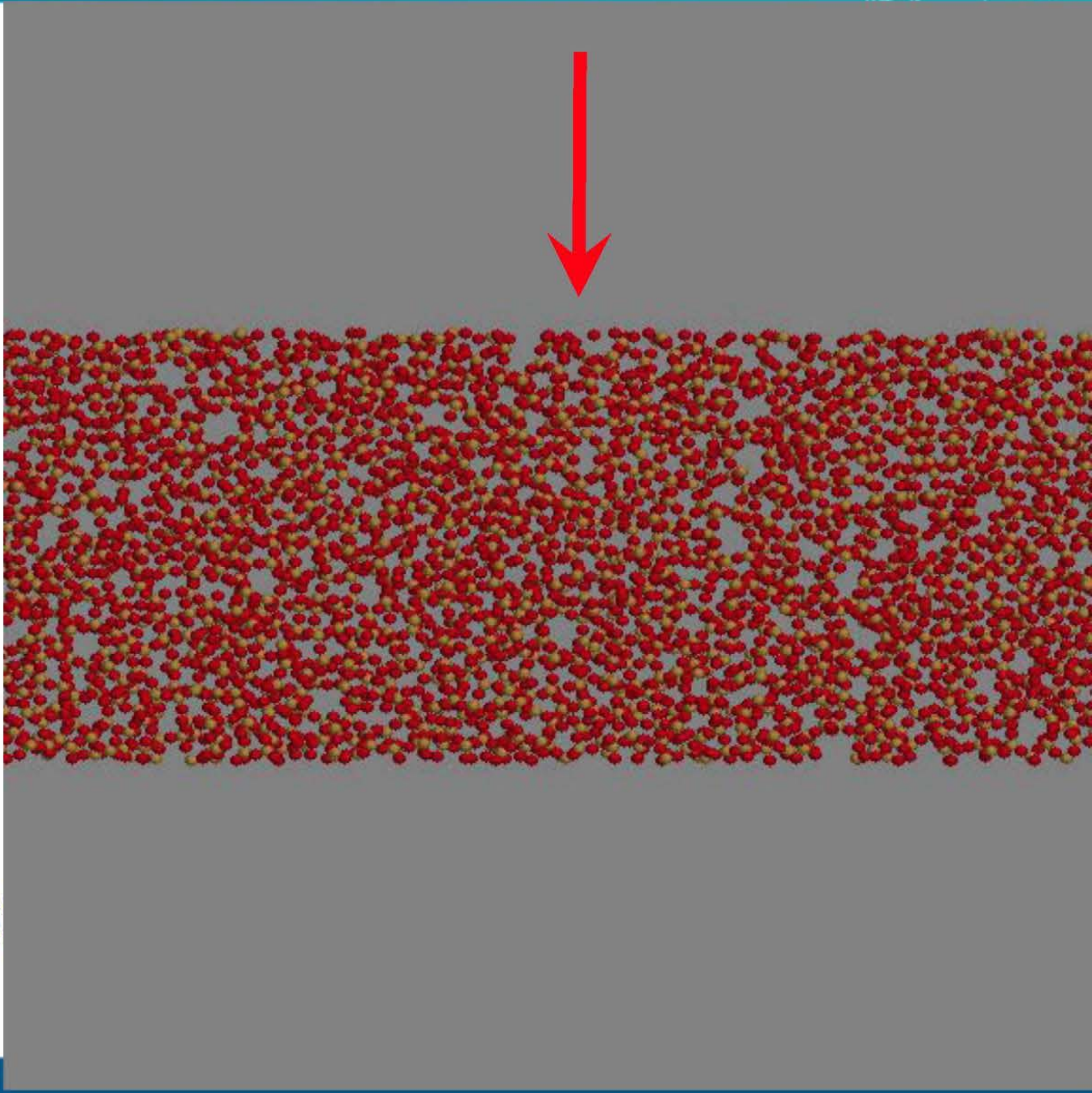
- Ion irradiation strongly affects the material
- Density change
- Refractive index
- Defects
- Network structure
- Electronic sputtering (surface)



MD

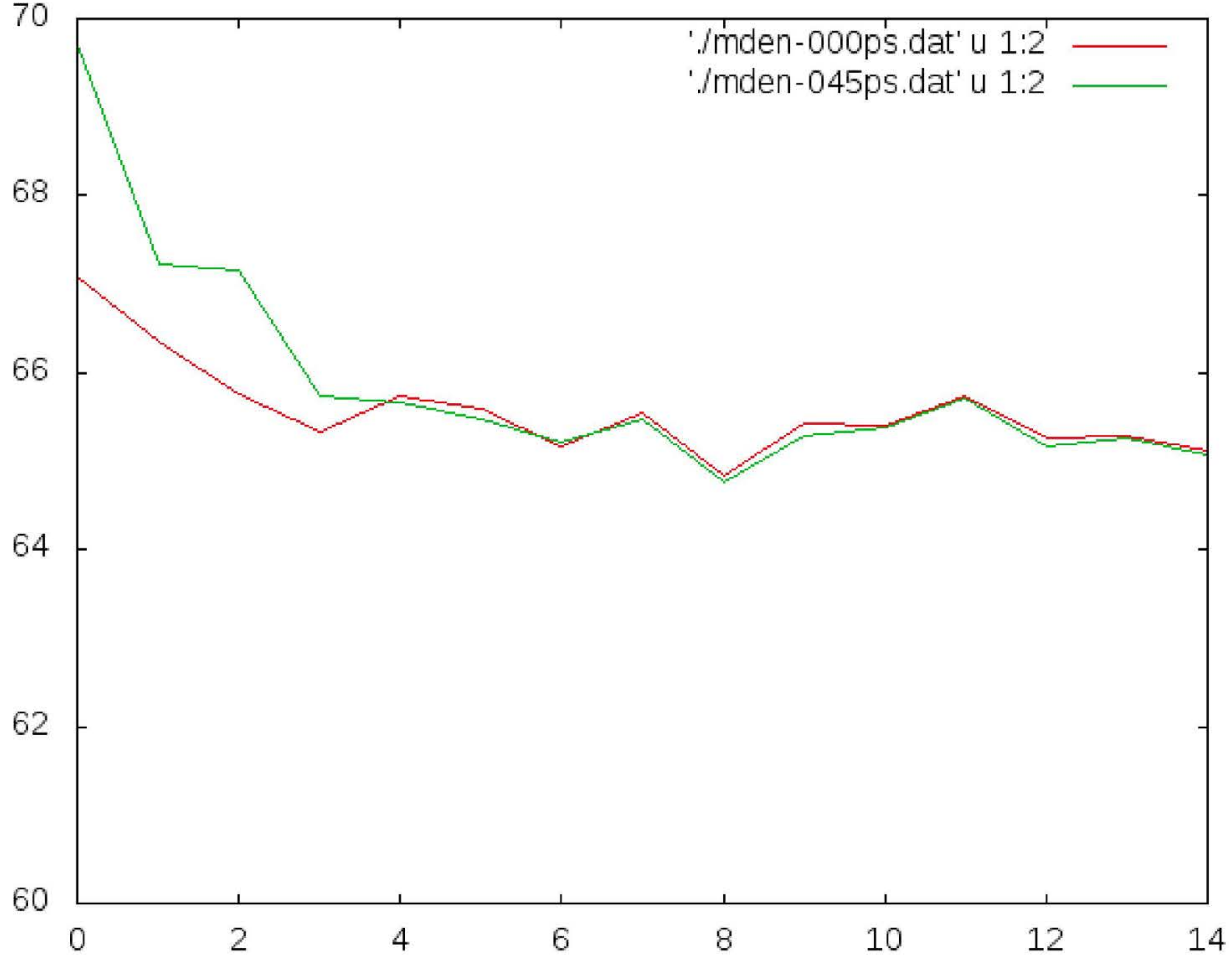
30 keV/nm

- Ion irradiation strongly affects the material
- Density change
- Refractive index
- Defects
- Network structure
- Electronic sputtering (surface)



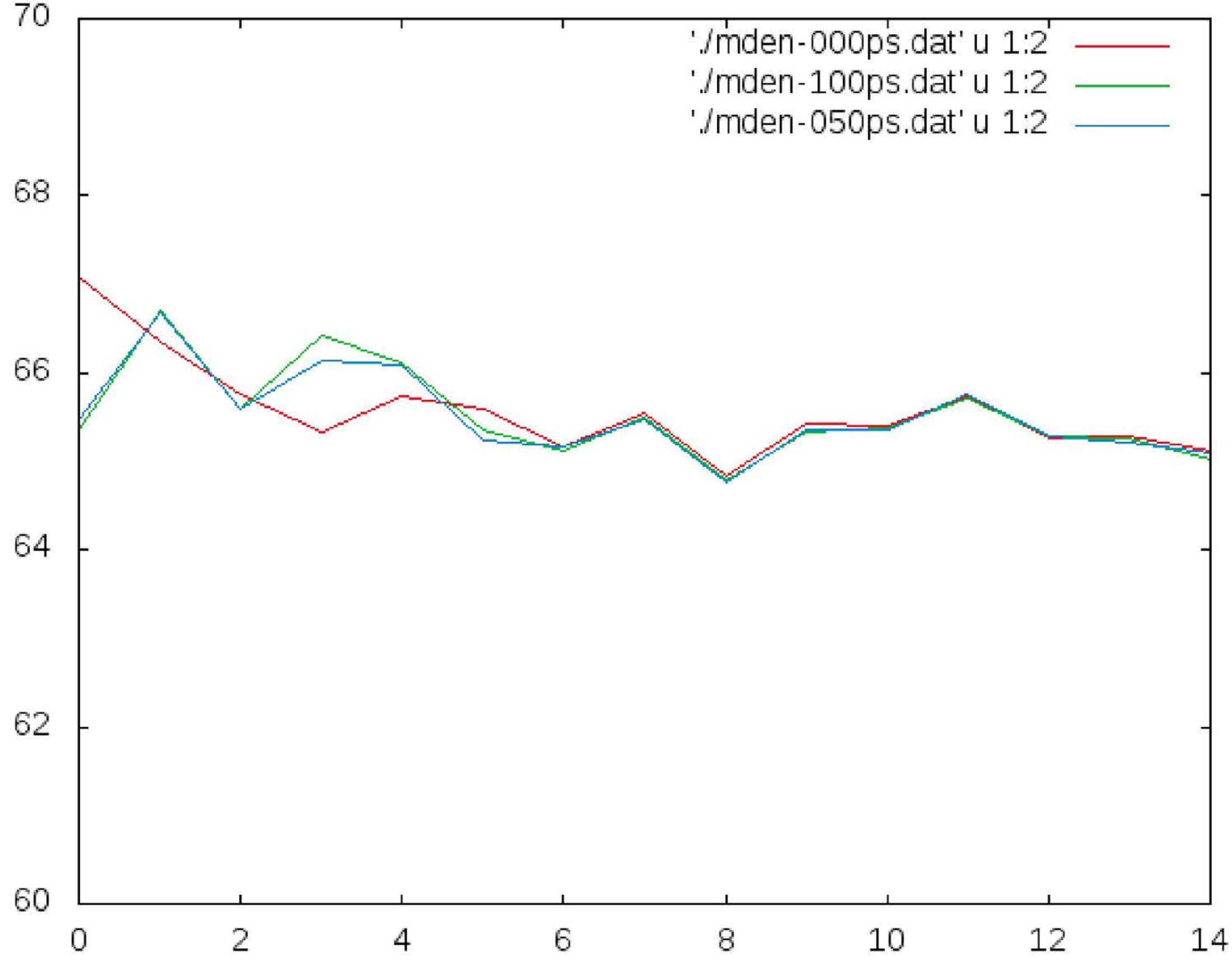
Density change

10 keV/nm



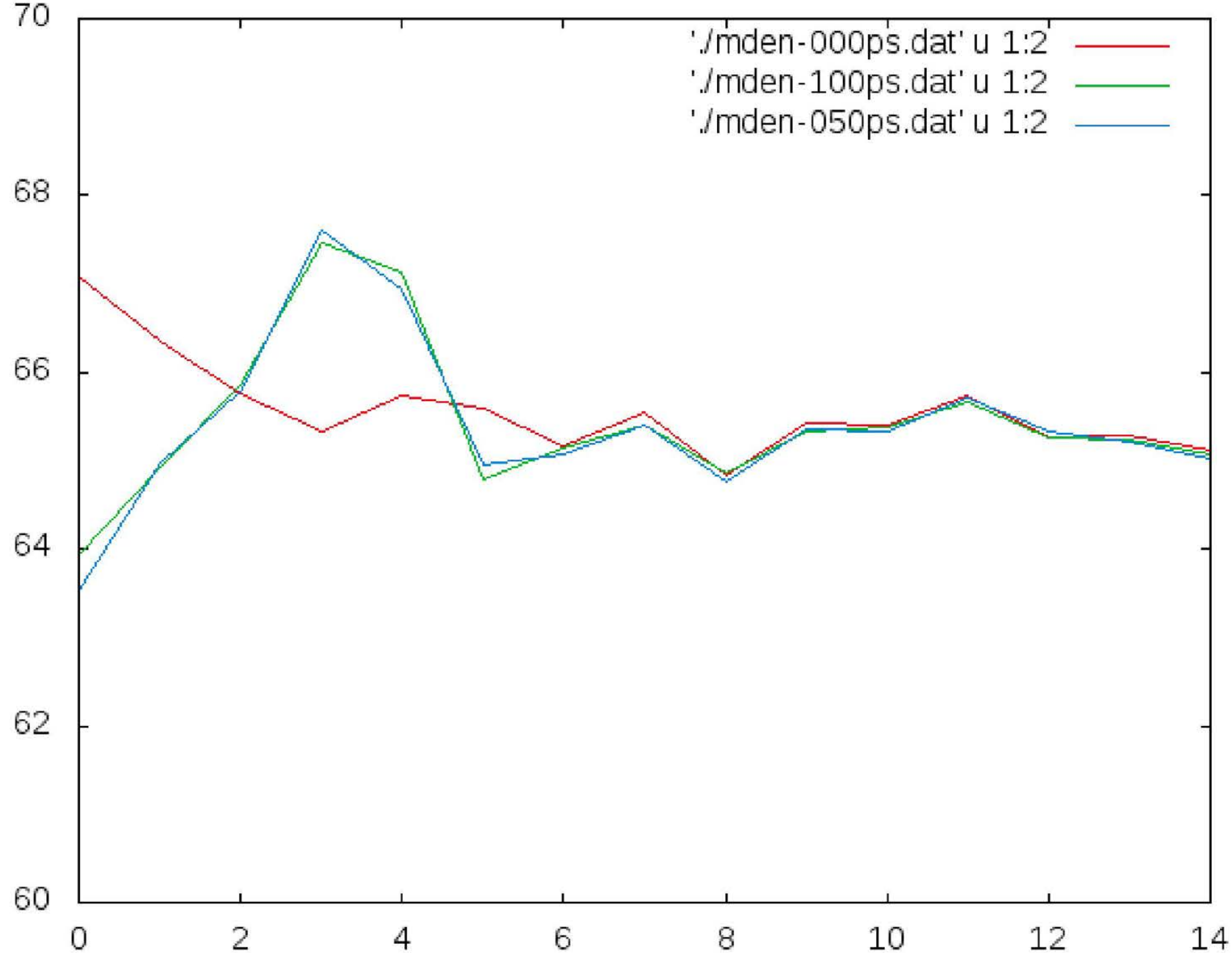
Density change

12 keV/nm



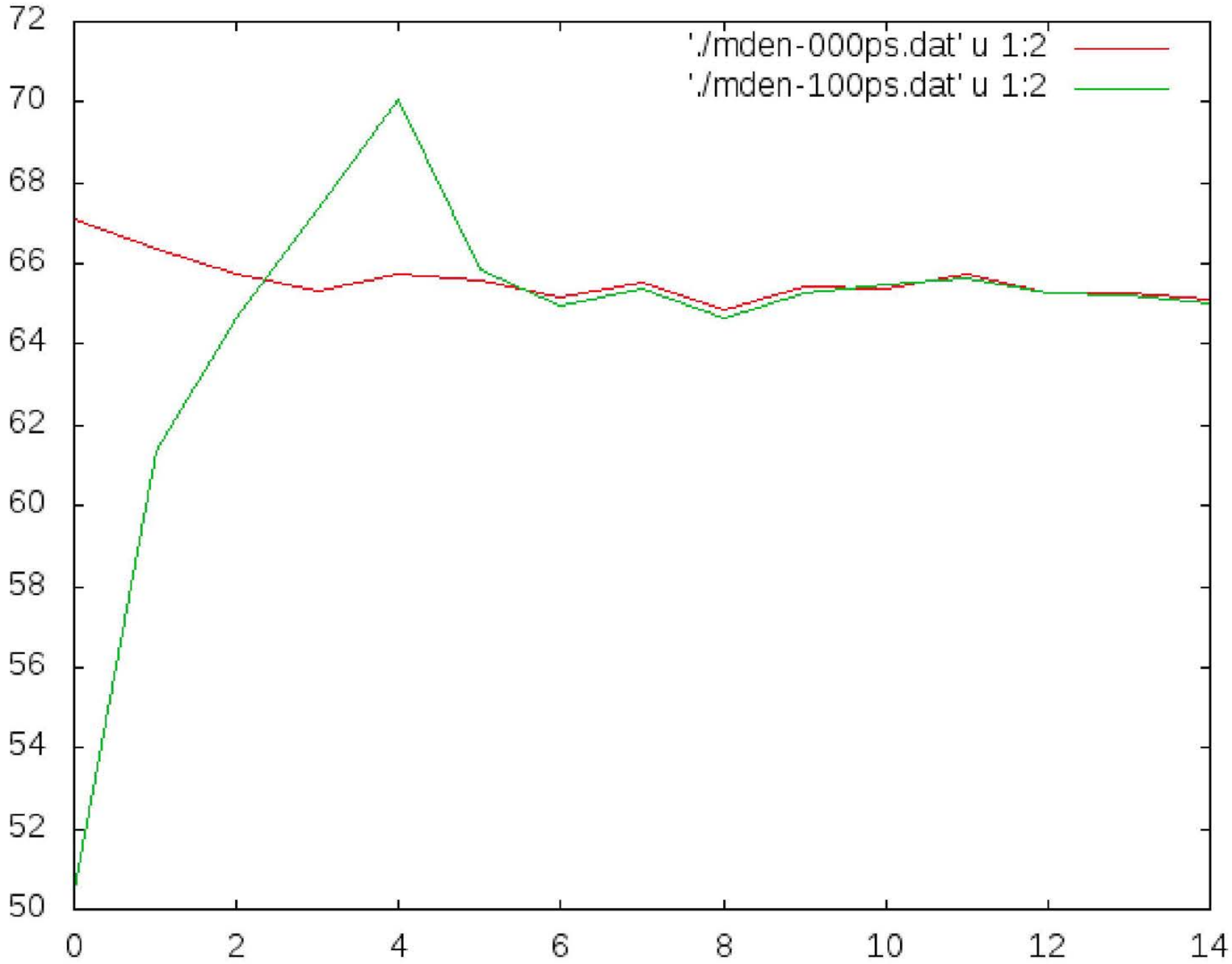
Density change

14 keV/nm



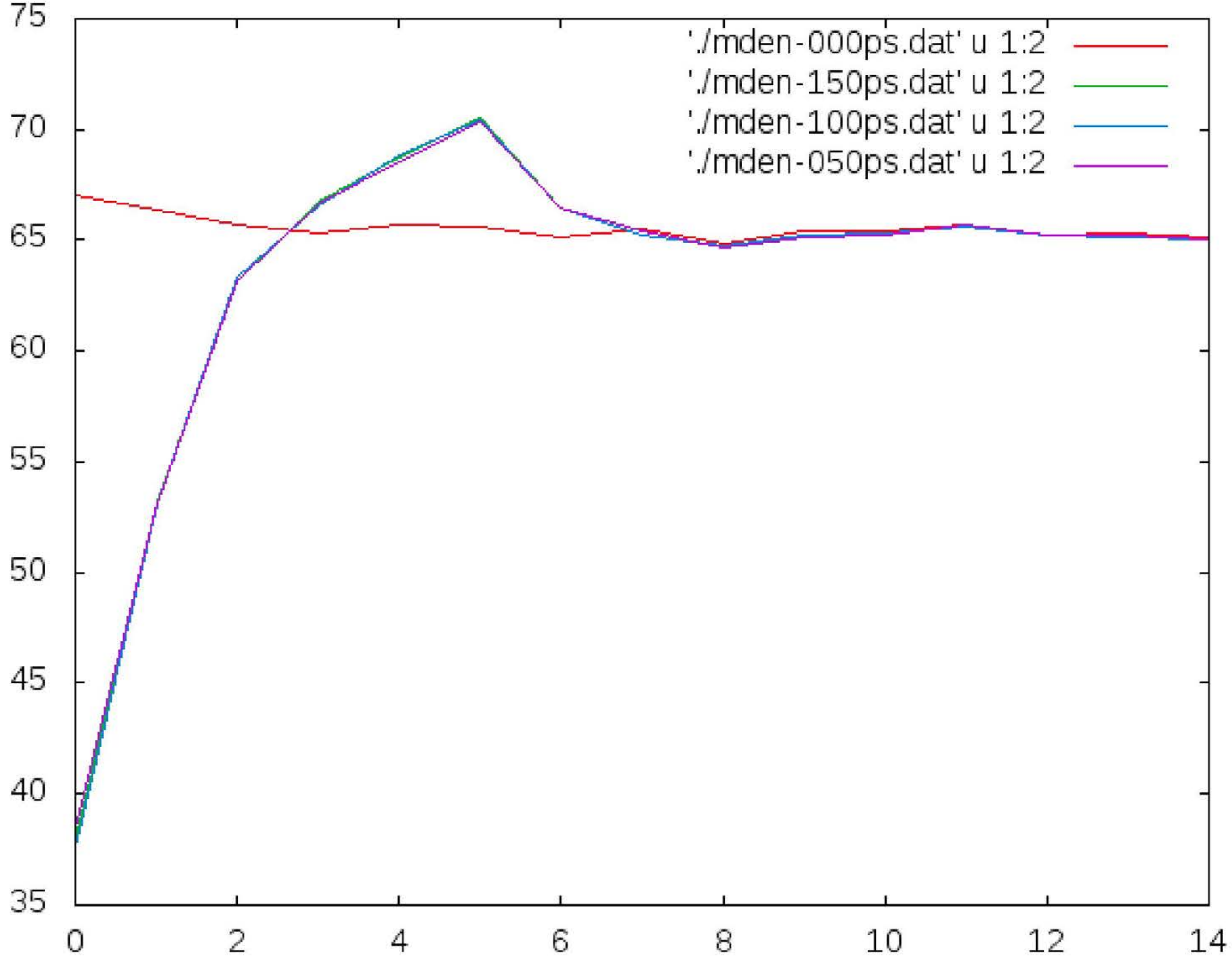
Density change

20 keV/nm



Density change

30 keV/nm



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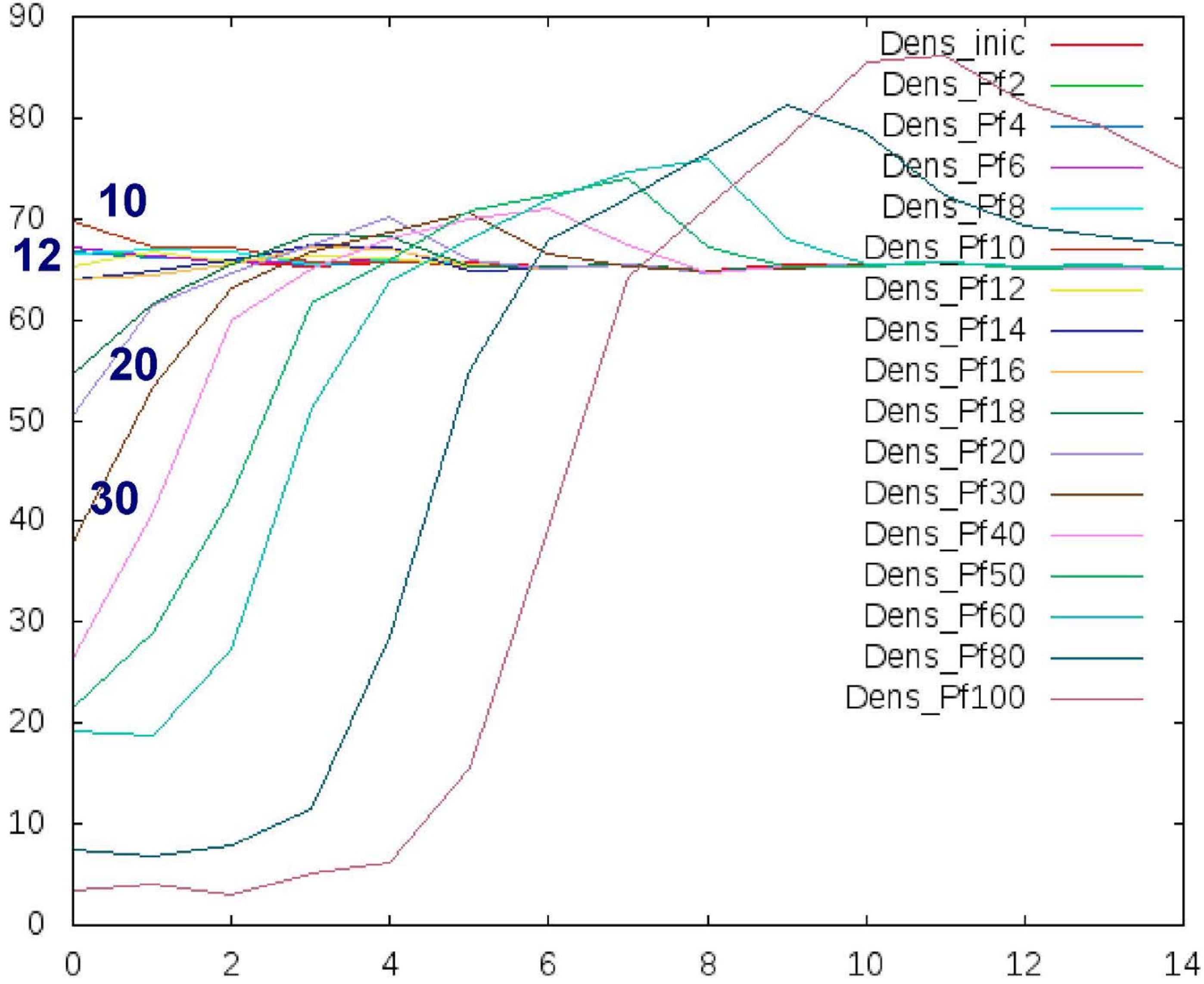
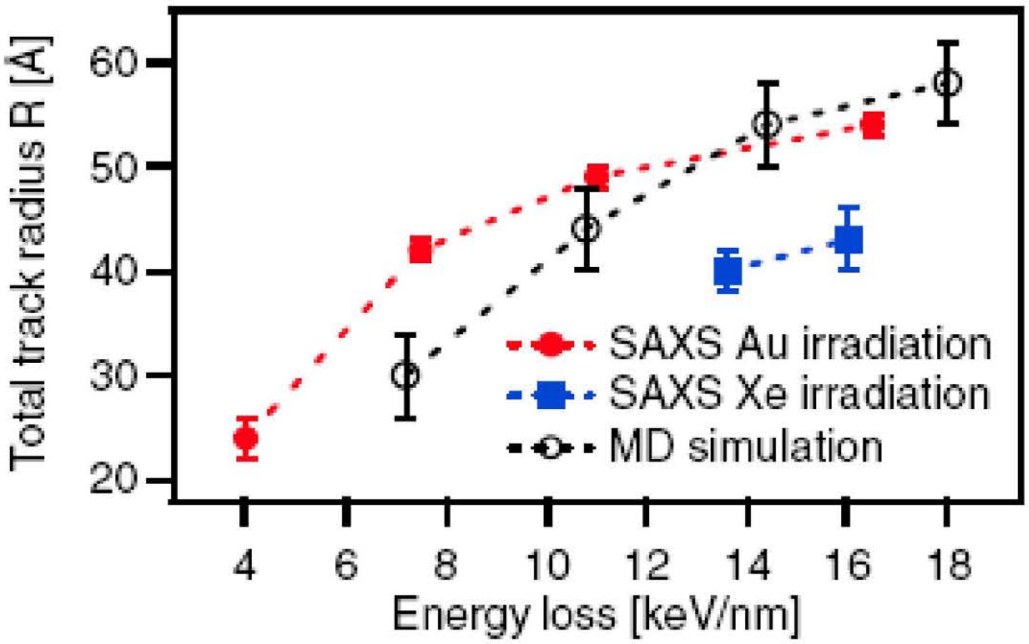
Density change



Density change

- Previous experimental and MD work show similar effects



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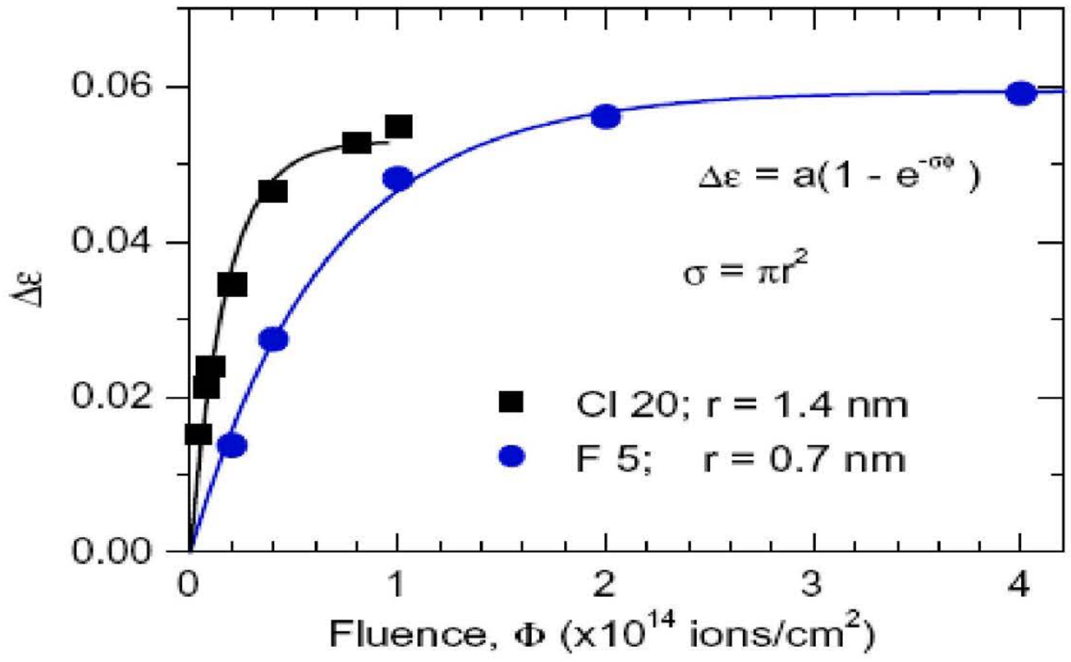
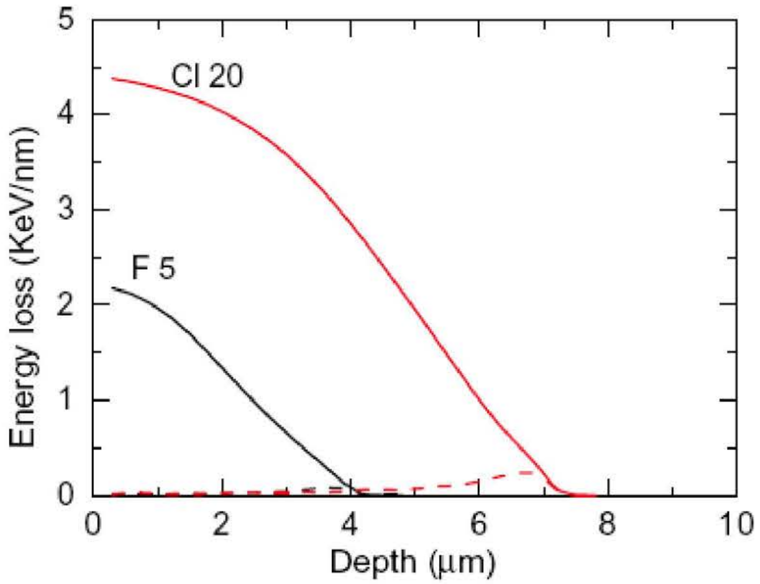
Optical measurements

- Low ion energy leads to guided modes by track overlapping





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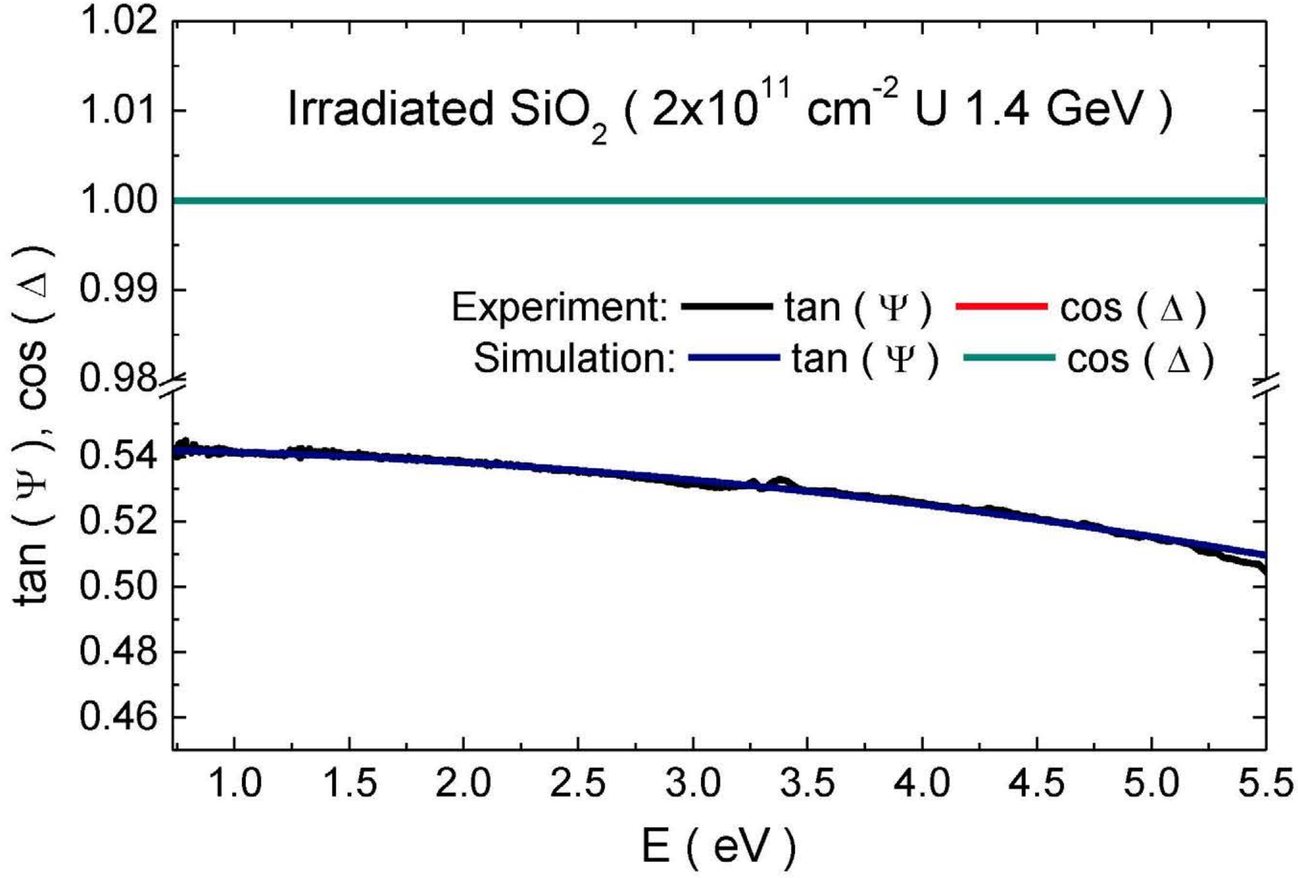
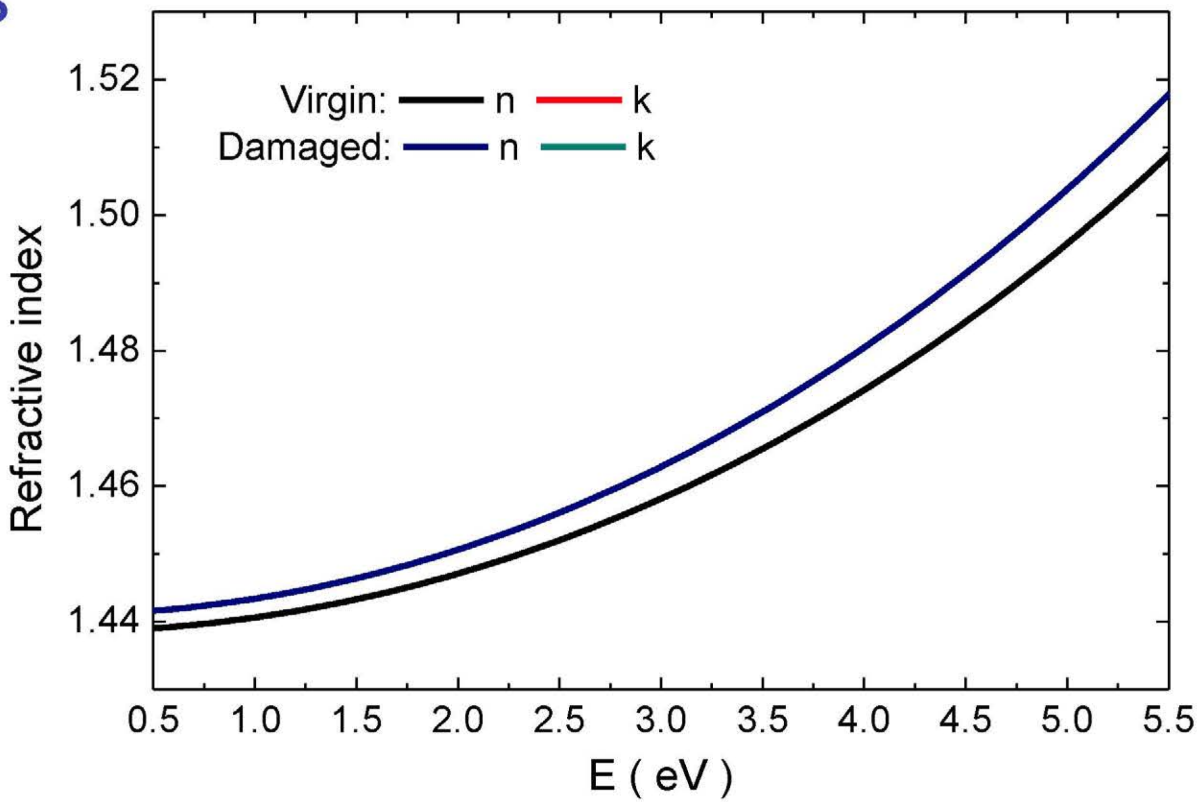
Experimental results

Silica sample
U 1.4 GeV
S_e = 35 keV/nm
$2x10^{11}$ ions/cm^2

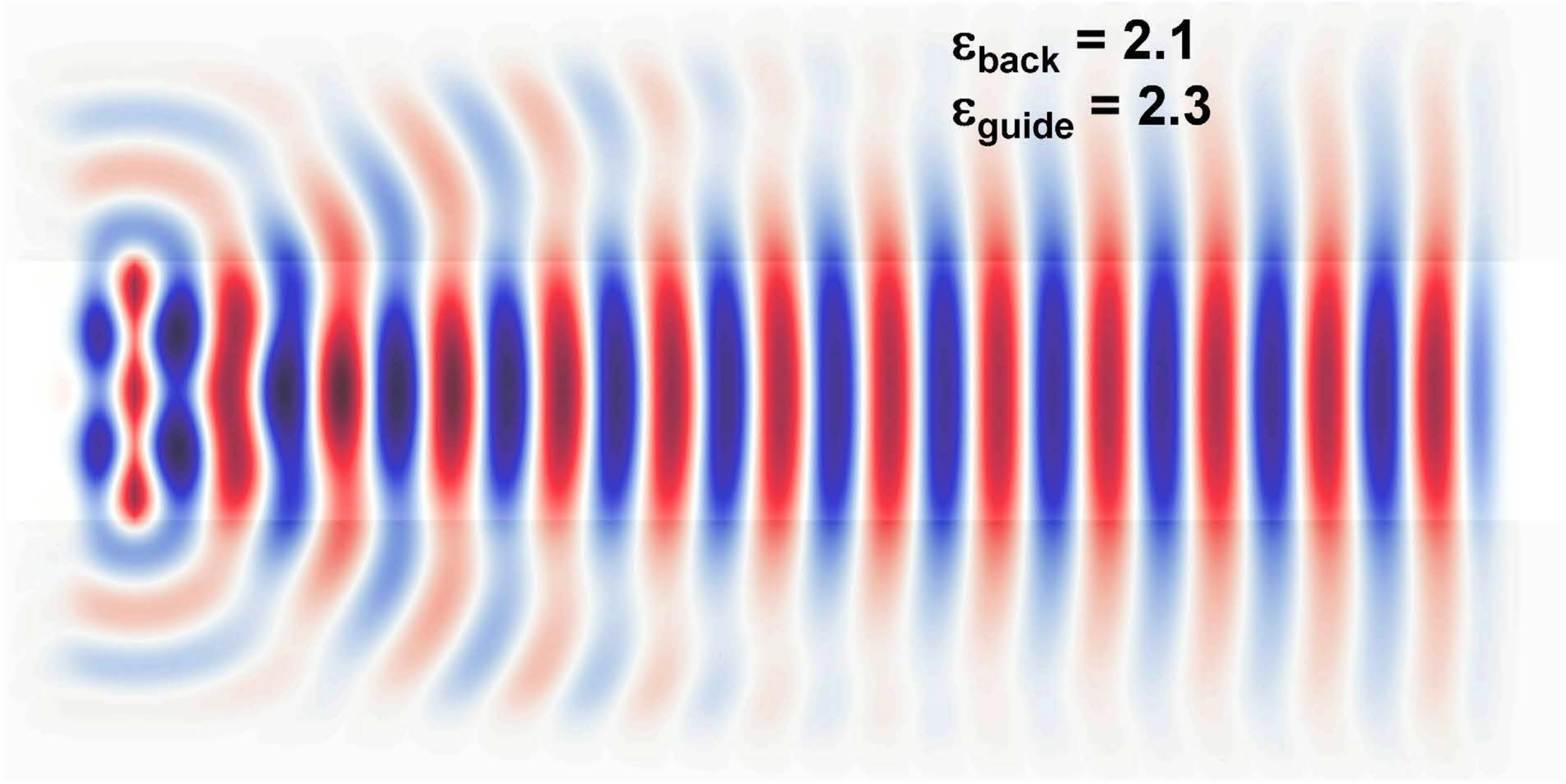


Optical measurements

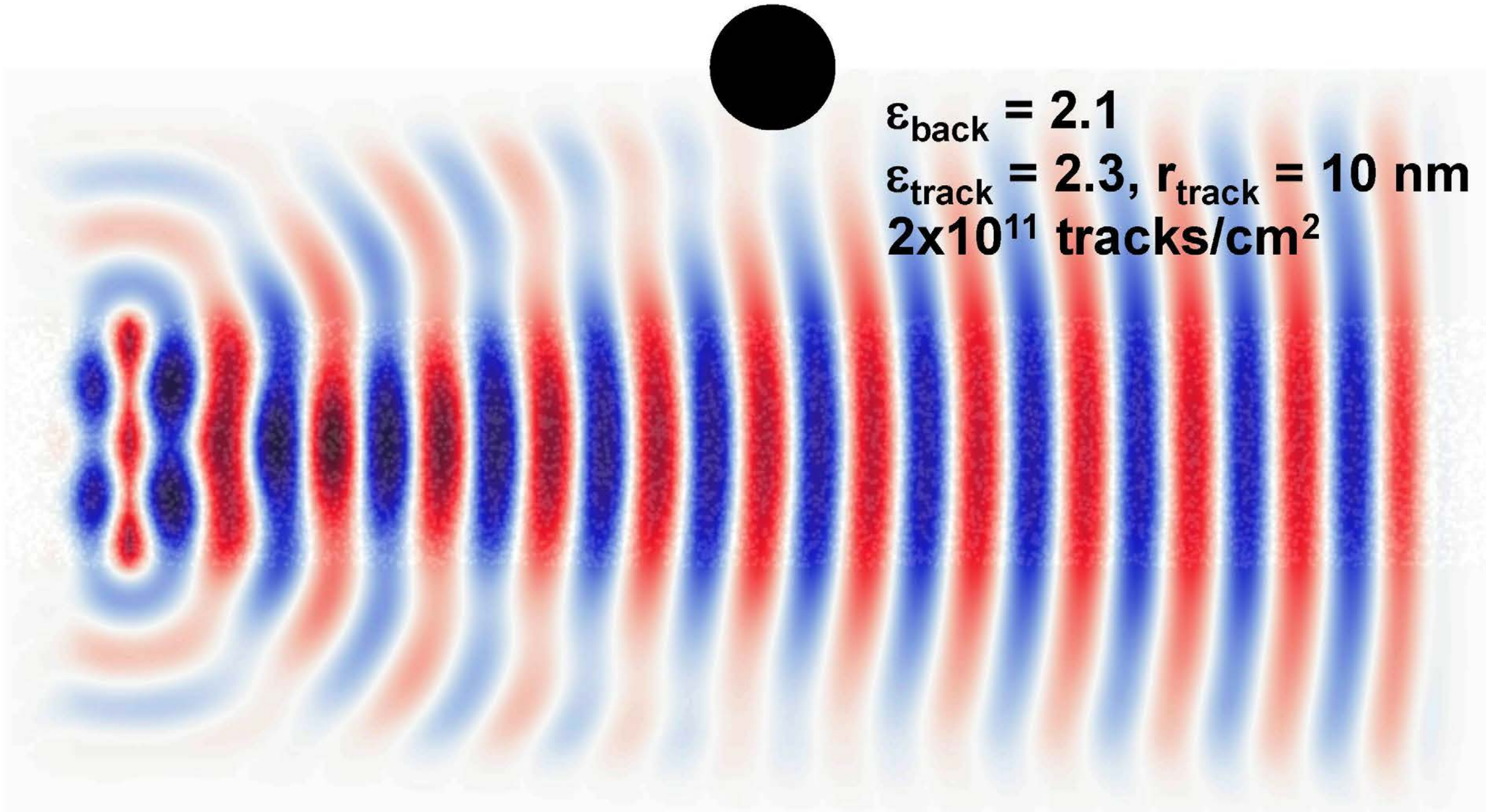
- High energy ions produce large complex tracks
- The result is an effective medium able to guide modes



Full guide (FDTD MEEP)



Solid tracks (FDTD MEEP)



ε_{back} = 2.1
ε_{track} = 2.3, r_{track} = 10 nm
$2x10^{11}$ tracks/cm^2

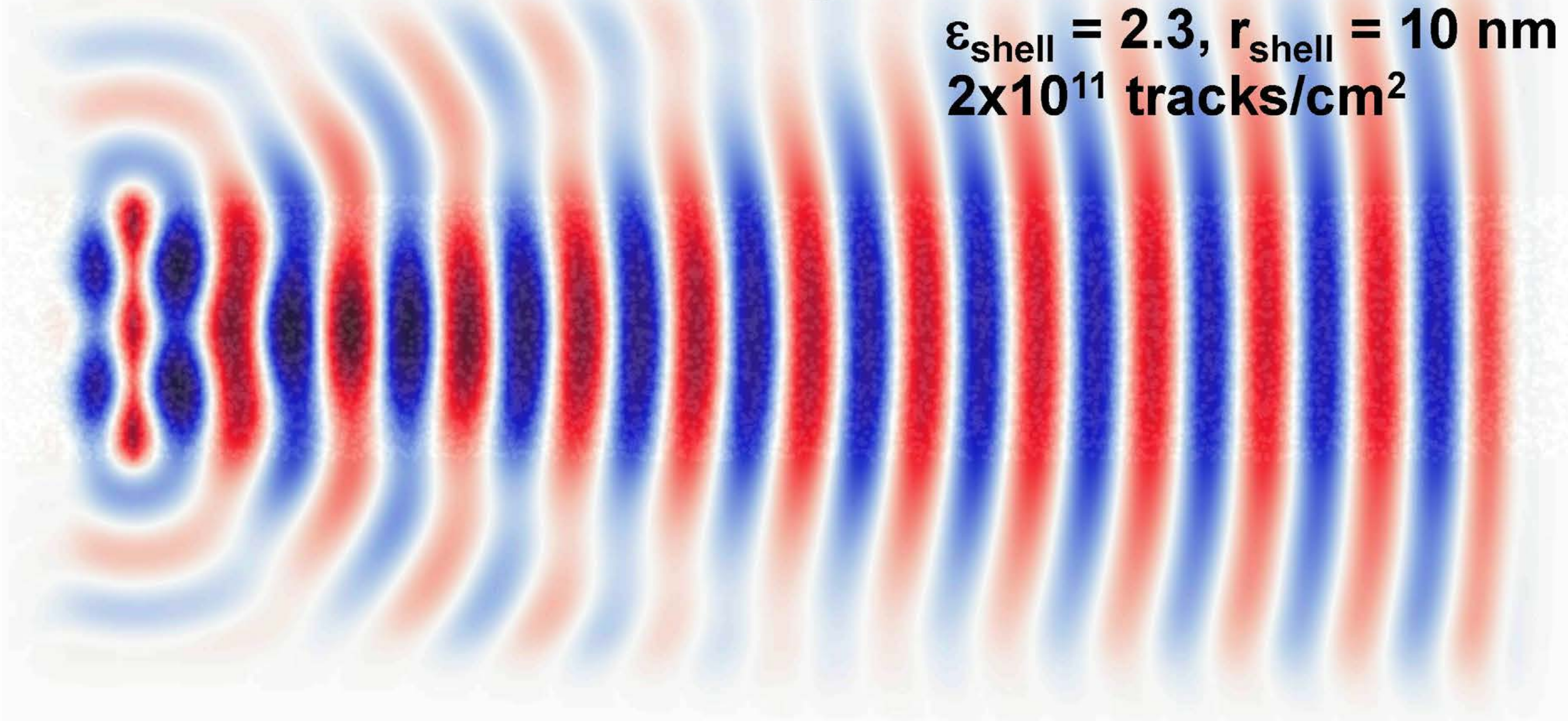
Core-shell tracks (FDTD MEEP)

ε_{back} = 2.1

ε_{core} = 1.8, r_{core} = 4 nm

ε_{shell} = 2.3, r_{shell} = 10 nm

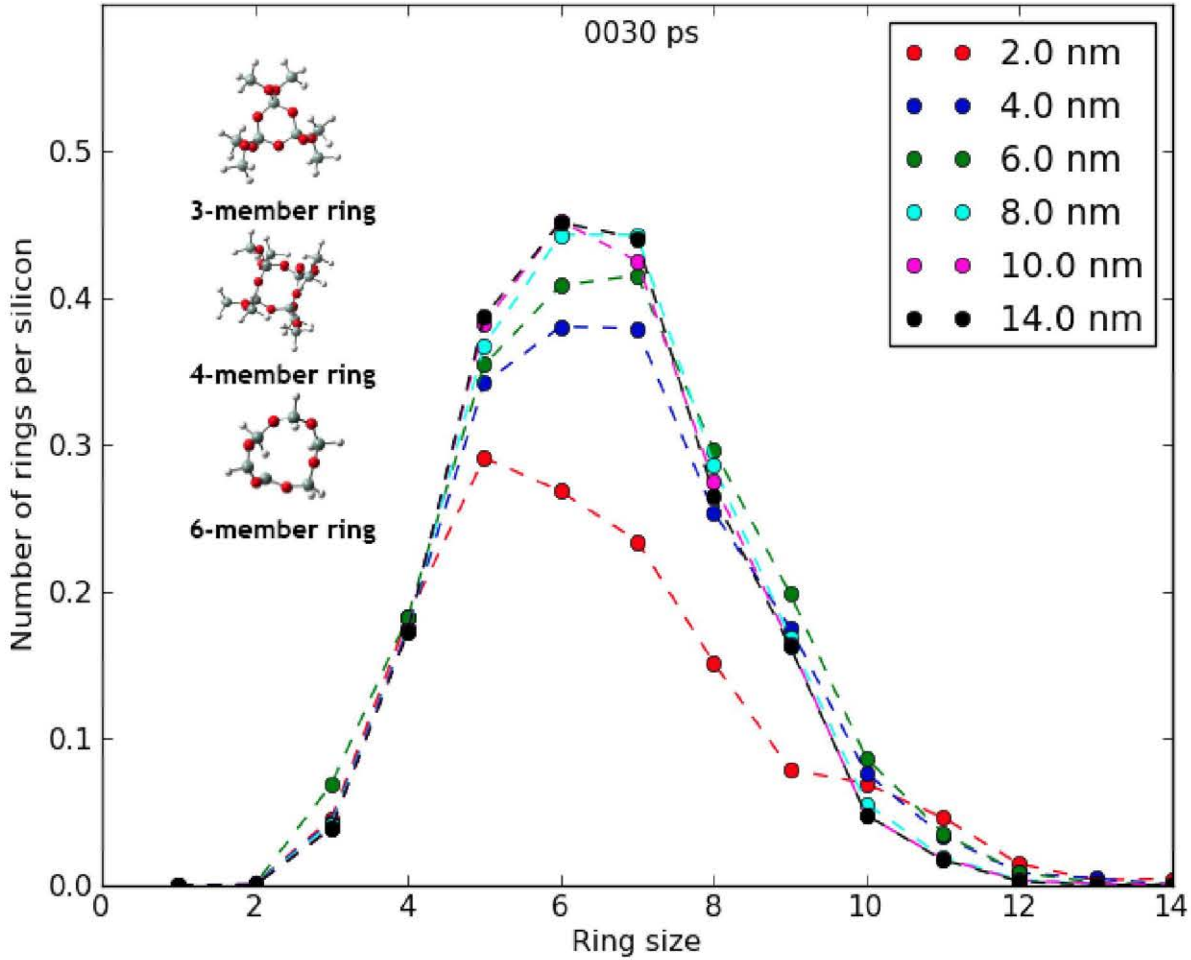
2×10^{11} tracks/cm^2



Network

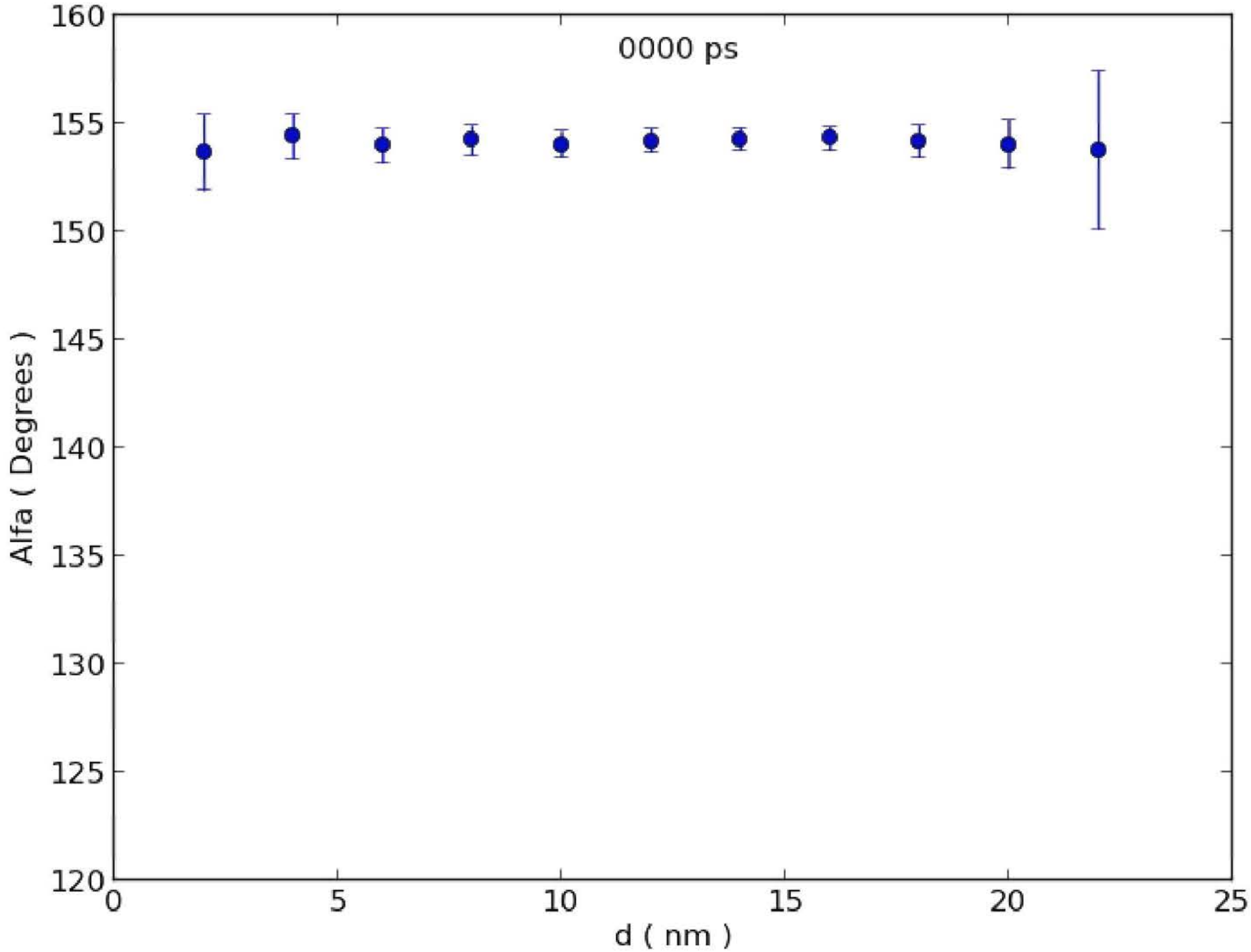
- Ring distribution
- Raman effect

30 keV/nm



Angles

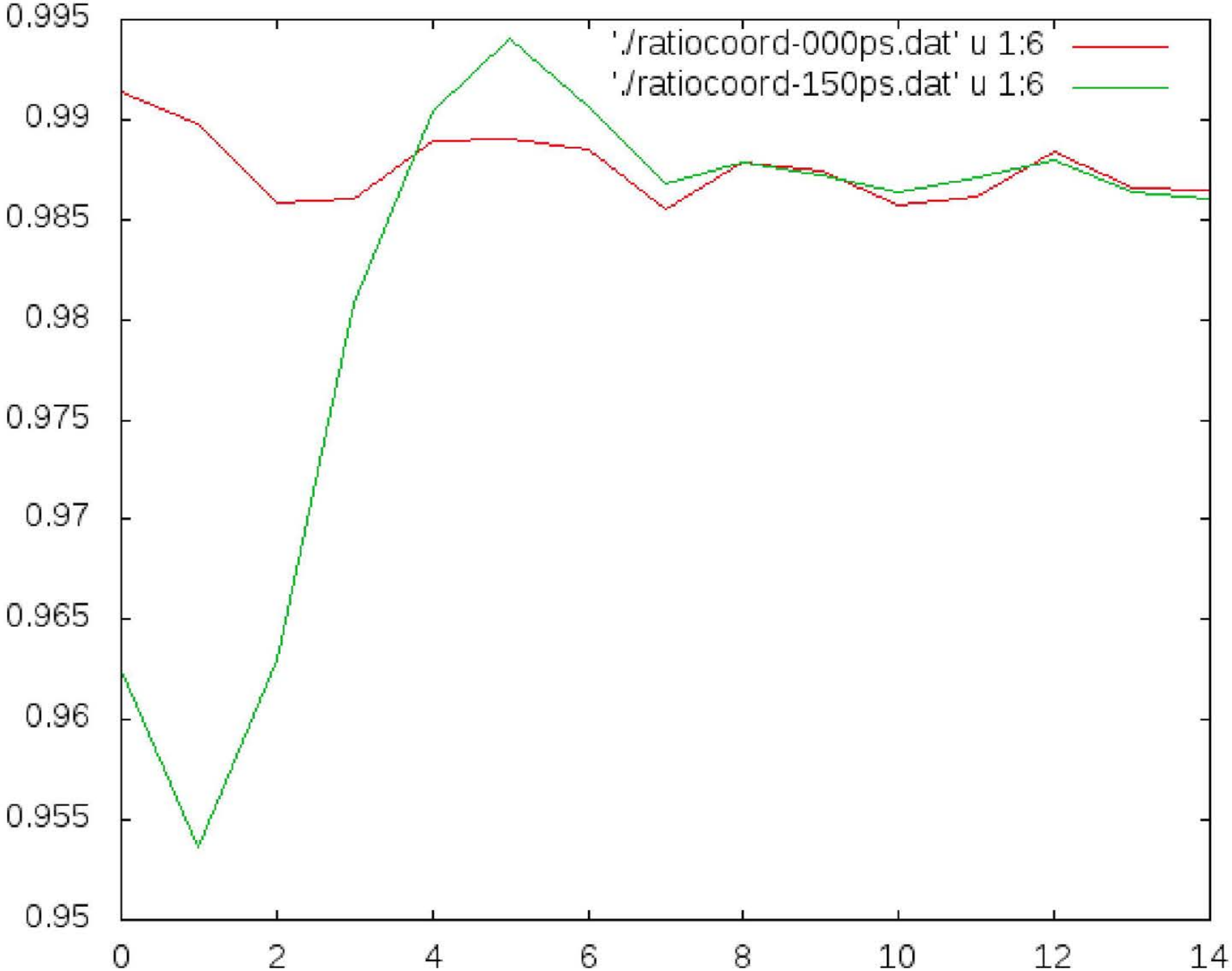
30 keV/nm



Defects

30 keV/nm

- At high s
  dramma
- Resultir



Defects

- At low stopping power the bond structure changes but it recovers
- We can not quantify permanent bond rupture fraction
- Therefore, the origin of permanent defects is unclear

Conclusions

- In order to study thermal effects we have simulated electronic excitation by MD
- Thermal effects on structure, density and defect generation have been identified
- Experiments and FDTD calculations with input from MD show that the tracks are compatible with mode guiding and therefore with refractive index increase
- Defect generation with high stopping power ions can be explained by thermal effects

Thank you