Radiation damage in the electronic regime

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SiMAF: Simulations in Materials Science, Astrophysics, and Physics

https://sites.google.com/site/simafweb

Non-adiabatic dynamics and radiation damage in nuclear materials

ICTP-IAEA, Trieste

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COLLABORATORS:

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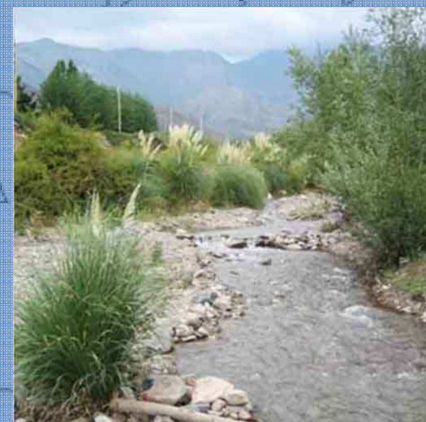
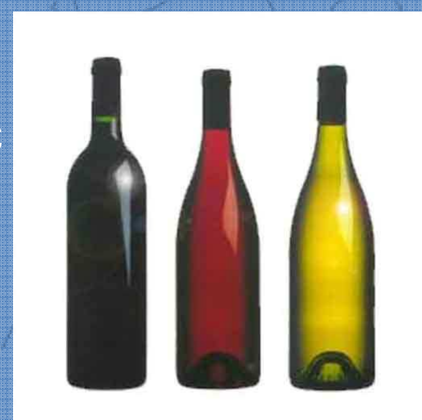
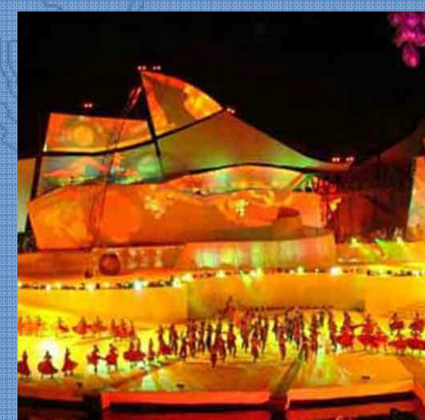
MENDOZA, LAND OF THE SUN AND THE GOOD WINE



Malbec

Top 2 harvest festival (Nat Geo 2011)





OUTLINE

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- Background and Introduction
  - Track models
- Molecular Dynamics (MD) of damage in the electronic regime
  - Thermal Spikes, Two Temperature Models and Coulomb Explosions.
- Examples
  - Electronic sputtering, track formation: defects, phase change, craters & bumps.
- Conclusions and future outlook

Ion-solid interaction in the electronic regime

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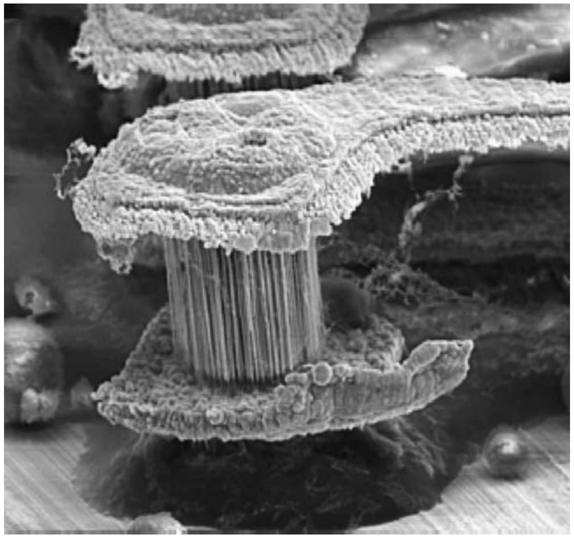
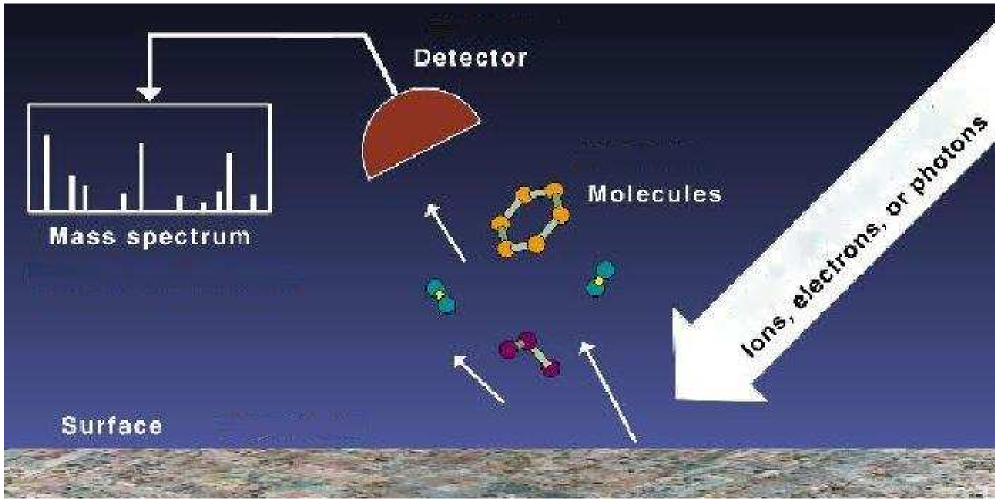


Microwires filling etched ion tracks
Toulemonde et. al, NIMB **216** (2004) 1.



Desorption of complex molecules
R.E. Johnson

Surface modification

Sputtering [Brown, 1980], adatom generation, craters, hillocks, nanopatterning, etc.

Bulk radiation damage

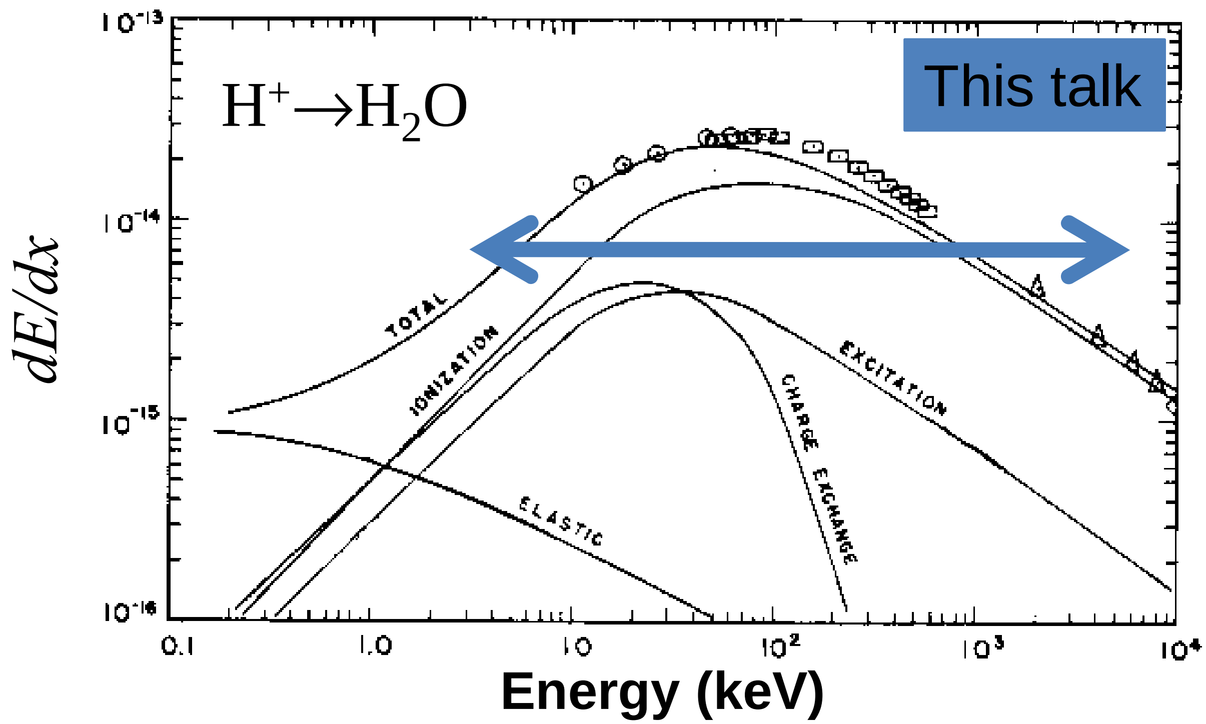
Defects, amorphization [Fleischer, Price & Walker 1965], re-crystalization, phase change, mixing, chemical changes,

***dE/dx* = Stopping Power.** Energy loss per unit path length

$$dE/dx = (dE/dx)_{nuc} + (dE/dx)_{elec}$$

$$(dE/dx)_{elec} = (dE/dx)_{ioniz} + (dE/dx)_{exc} + (dE/dx)_{ch\text{-}exch}$$

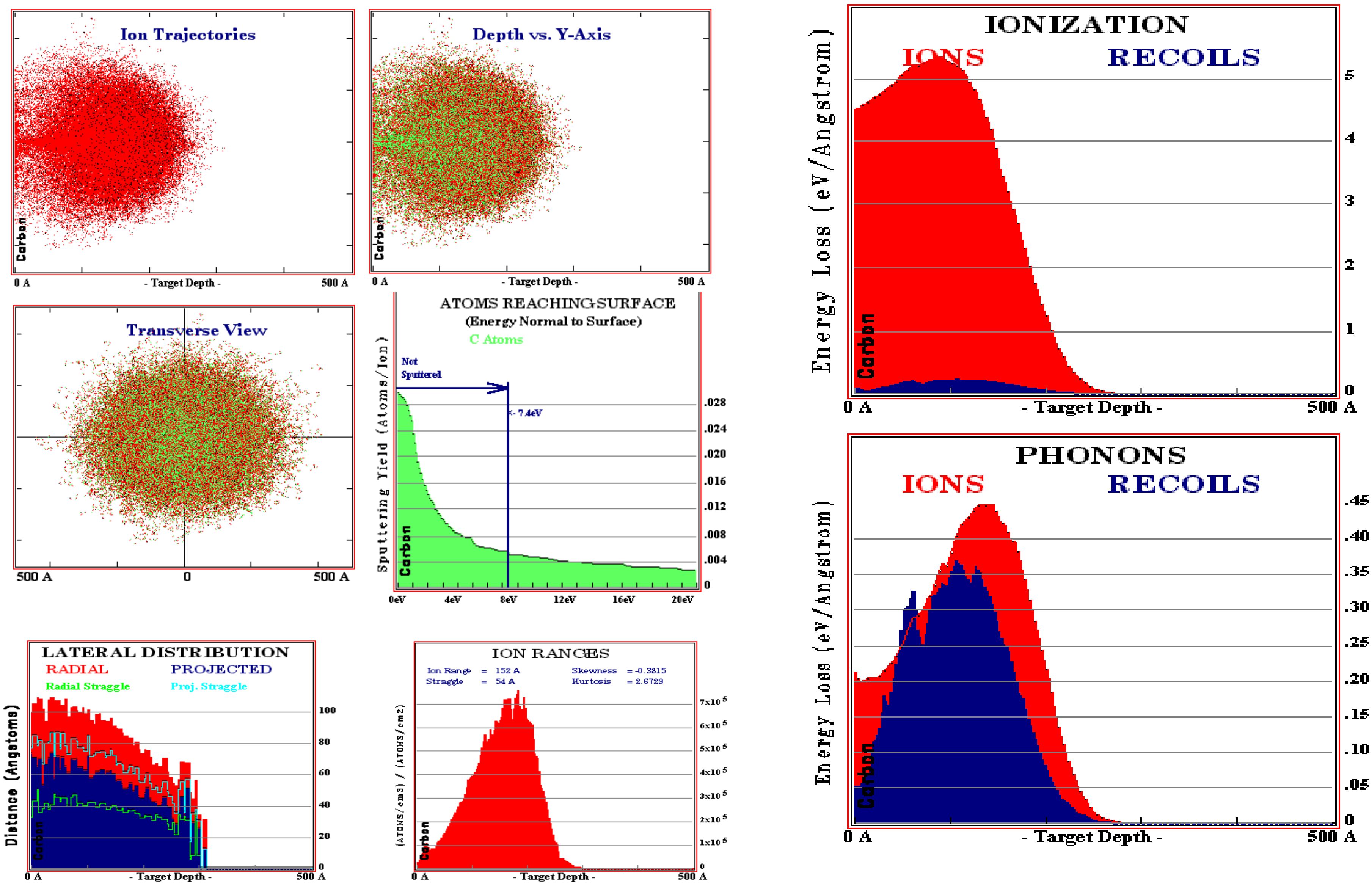
Stopping Cross Section: **S=** (*dE/dx*)/n
n is the density of the material



1 keV H⁺ → C

SRIM 2000 (Ziegler and Biersack) 10^4 ions

dE/dx=5.2 eV/Å, 90% electronic. Range=135 Å. Max at 80 keV



1 MeV H^+ ➔ C SRIM 2000 (Ziegler and Biersack) 10^4 ions

dE/dx=5.4 eV/Å, 99.9% electronic. Range=11.5 μm. Max at 80 keV

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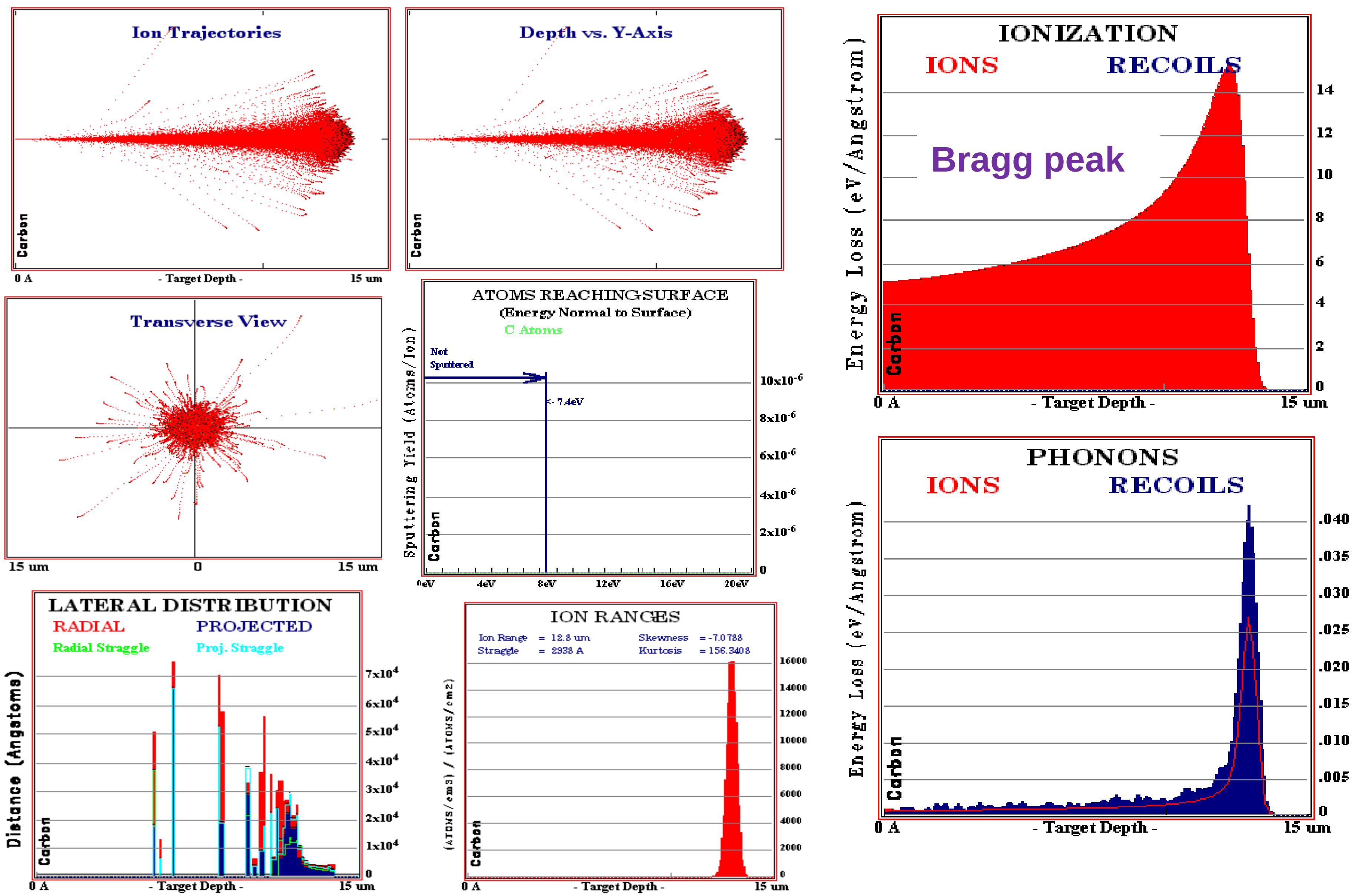
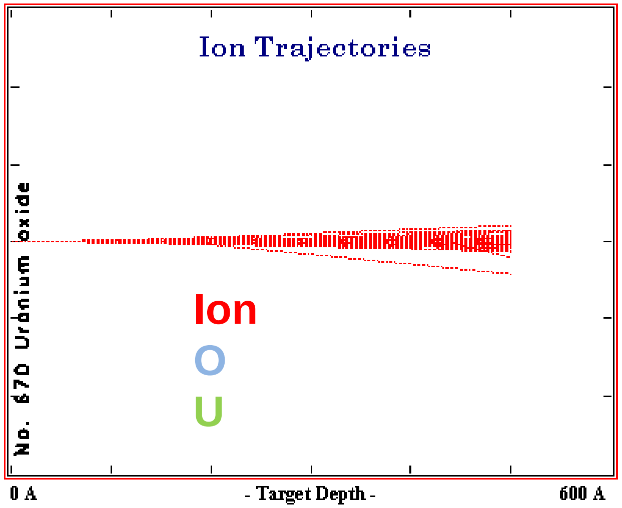
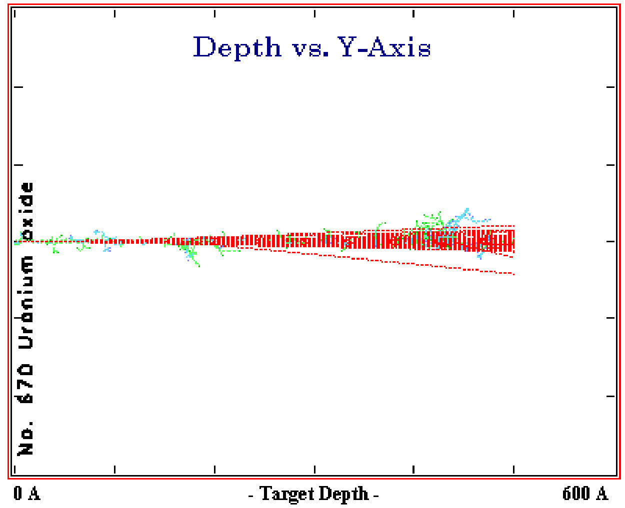
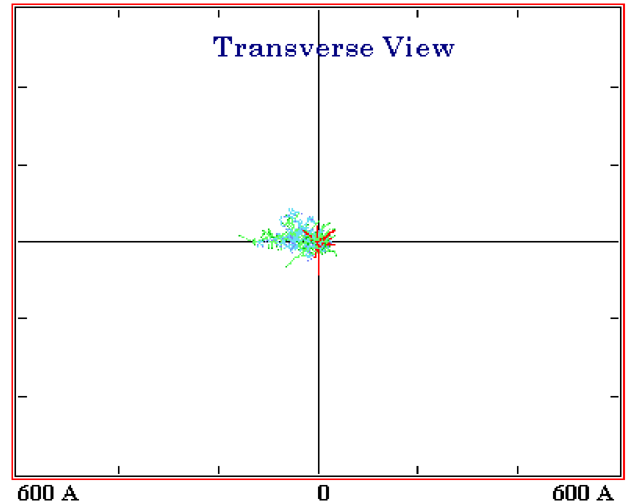


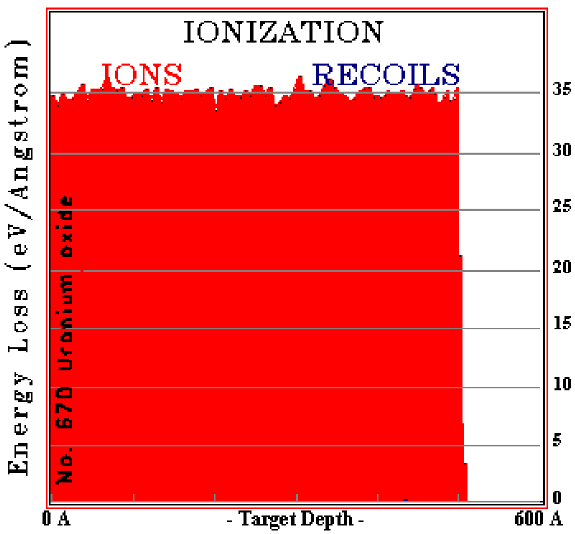
4 MeV He→ UO_2 SRIM 2006 (Ziegler and Biersack) 10^2 ions

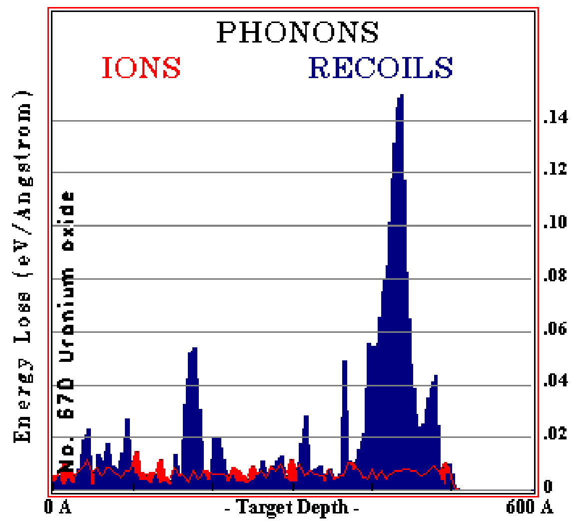
This is a quick test. 100 ions too few for MC











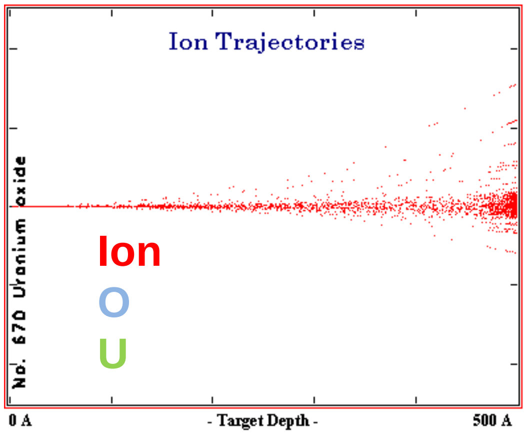
Approximation of a cylindrical track of electronic excitations with constant $(dE/dx)_{el}$ works well for the first 0.5 μm

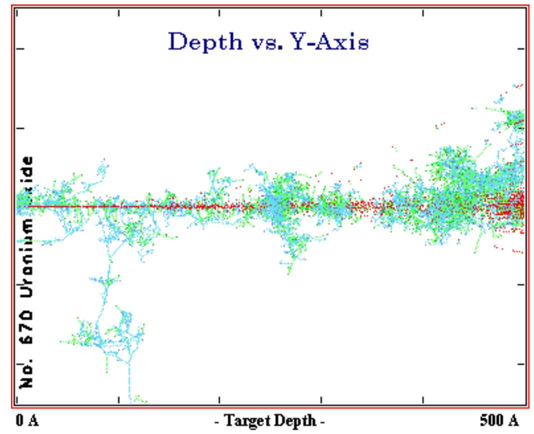
$(dE/dx)_{el}$=3.5 keV/nm, $(dE/dx)_{nuc}$=0.014 keV/nm, R_p= 1.8 μm (0.4 μm straggling)

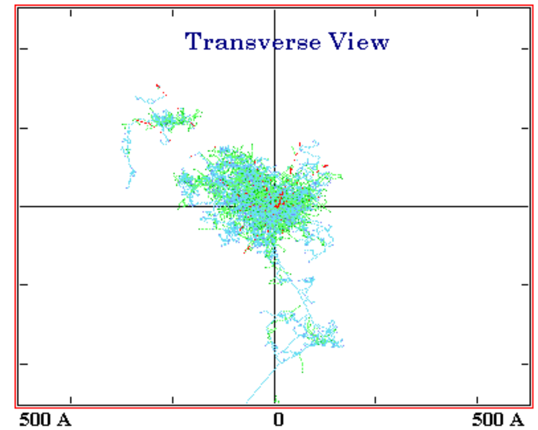
$(dE/dx)_{el}$ has maximum at 6.5 MeV

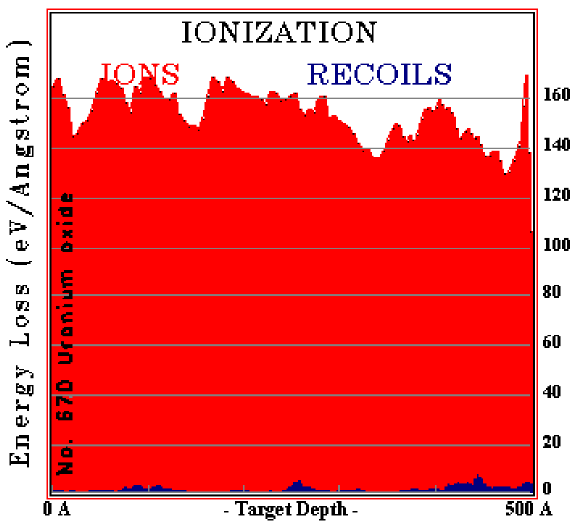
1 MeV O→ UO_2 SRIM 2006 (Ziegler and Biersack) 10^2 ions

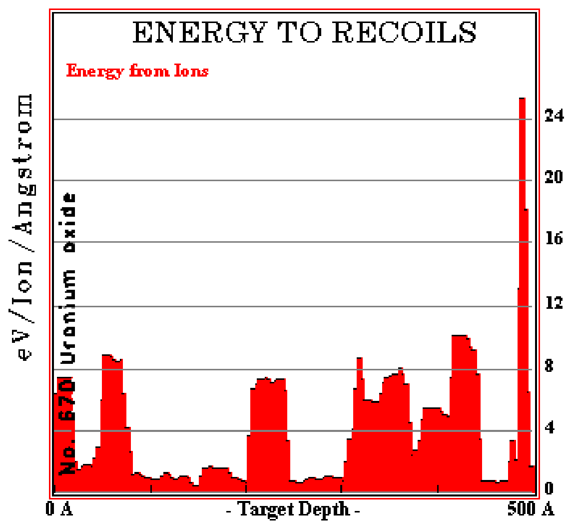
This is a quick test. 100 ions too few for MC











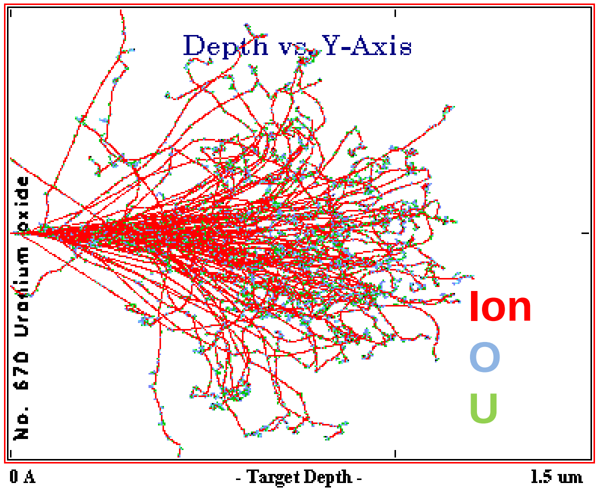
Approximation of a cylindrical track of electronic excitations with constant $(dE/dx)_{el}$ works OK for the first 0.5 μm

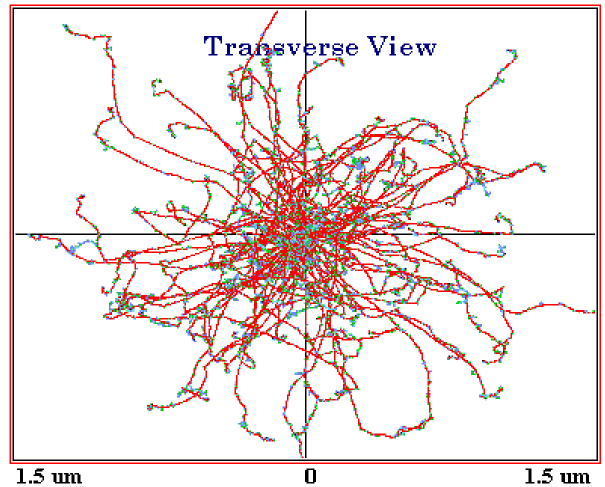
$(dE/dx)_{el}$=1.5 keV/nm, $(dE/dx)_{nuc}$=0.038 keV/nm, R_p= 0,8 μm (0.2 μm straggling)

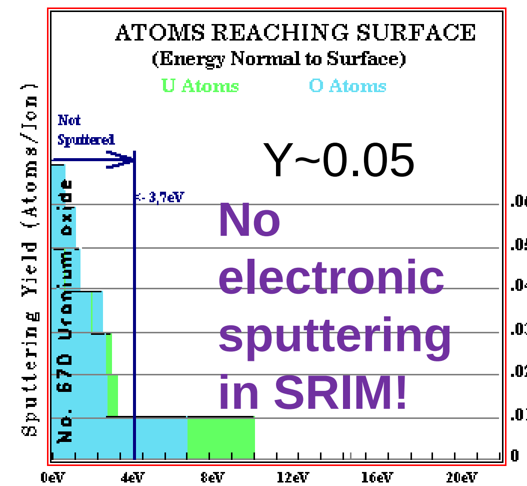
$(dE/dx)_{el}$ has maximum at 6.5 MeV

1 MeV O→ UO_2 SRIM 2006 (Ziegler and Biersack) 10^2 ions

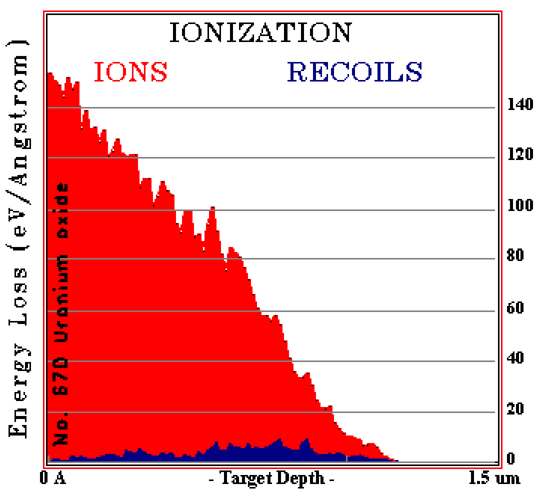
This is a quick test. 100 ions too few for MC

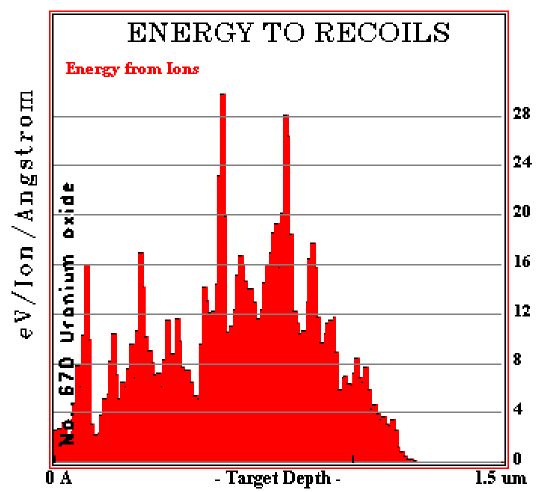


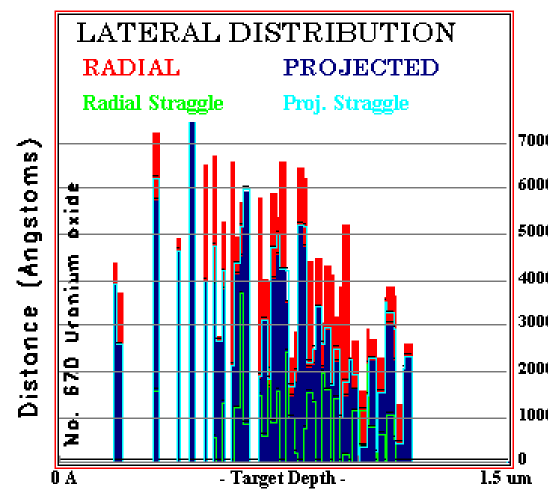




93% electronic stopping



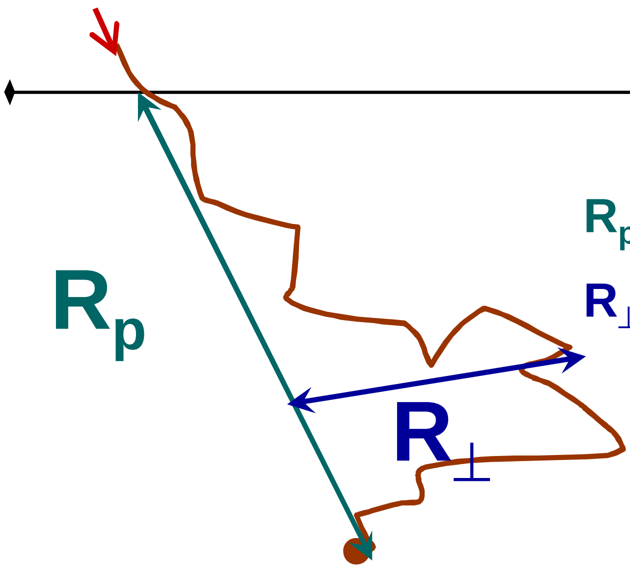




$(dE/dx)_{el}$=1.5 keV/nm, $(dE/dx)_{nuc}$=0.038 keV/nm, R_p= 0,8 μm (0.2 μm straggling)

$(dE/dx)_{el}$ has maximum at 6.5 MeV

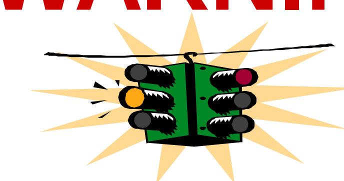
Ion Range, or where does an ion stop?



R_p = *Projected Range*

$R_\perp$ = *Perpendicular Range*

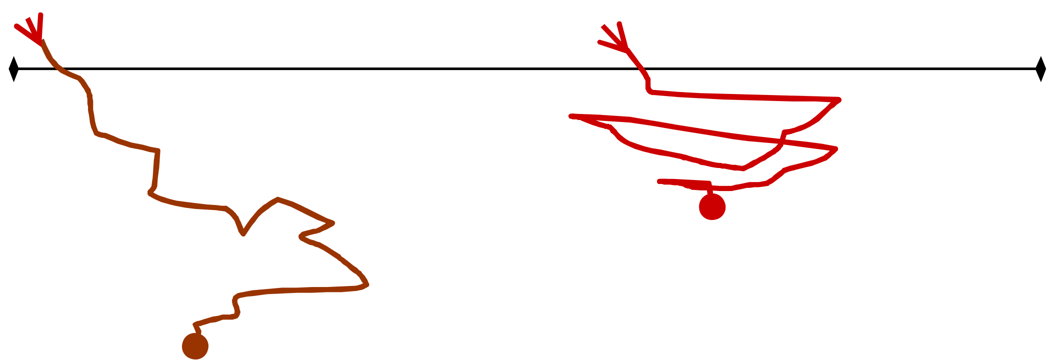
WARNING!!



Stopping and Range

have statistical fluctuations!!!

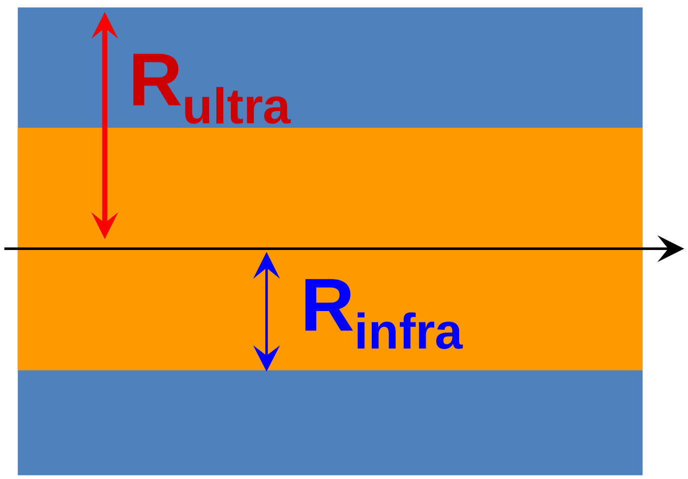
Sometimes the largest fluctuations may determine the final outcome



$$\mathbf{R} = \int |dE/dx|^{-1}\, dE$$

Track dimensions and structure

Infra and Ultra Track

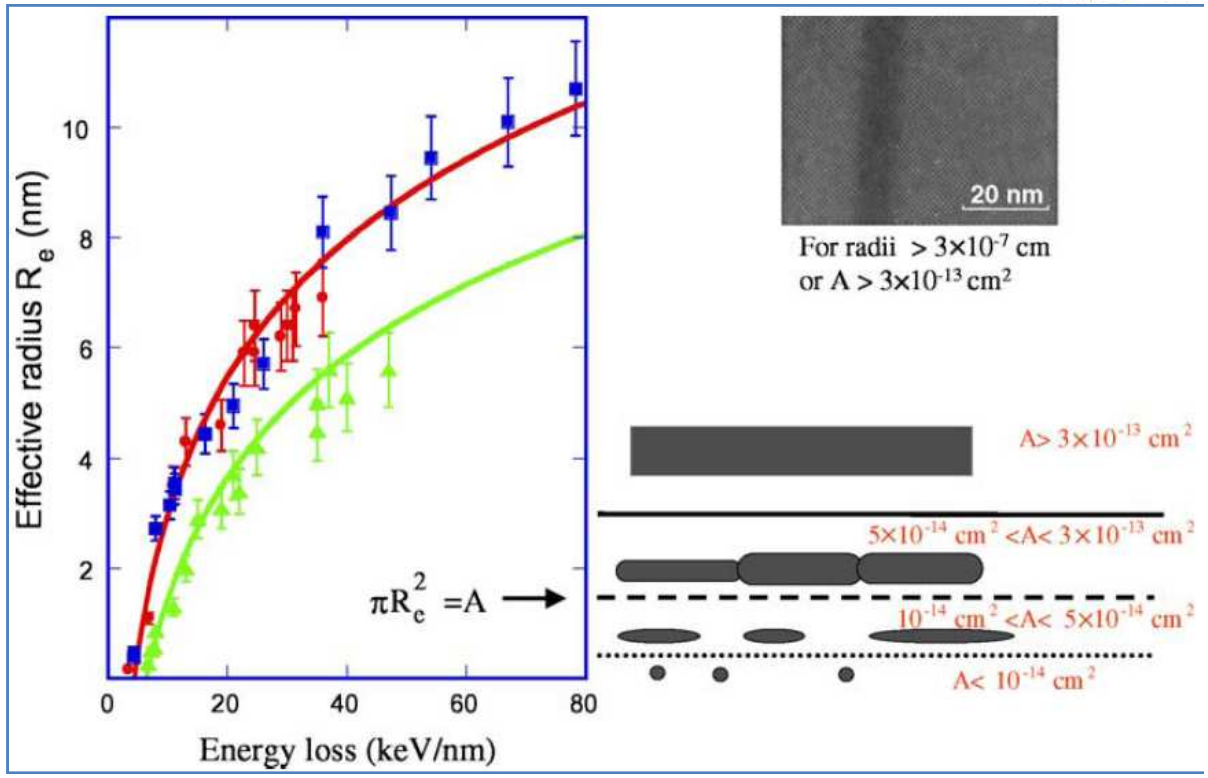


$R_{infra}=R_{core} \sim r_B \sim v/\omega_o$,
$h\omega_o$= first excitation energy

➔ Velocity effect: damage different for the same *dE/dx*

$R_{ultra} \sim$ maximum range of $\delta e^- \propto E_{ion}$

Johnson & Schou, *Mat. Fys. Medd. Dan. Vid. Selsk*. **43** (1993) 403.



Track radius R_e versus *dE/dx* for $Y_3Fe_5O_{12}$
Damage cross section: A= πR_e^2
Toulemonde *et. al*, NIMB **216** (2004) 1.

Not necessary to assume continuous track in MD (Schwen & Bringa, NIMB 2007)

"Effective" Stopping Power

$(dE/dx)_{\text{effective}} = \alpha f\, (dE/dx) = \eta\, (dE/dx)$; $\eta < 1$

$\alpha =$ *fraction deposited at the surface*

f = fraction that goes to relevant kinetic energy transfers, not spent in luminescence or in other excitations.

Nuclear Sputtering

$\alpha = \alpha(M_{\text{tar}}, M_{\text{proj}}, \Theta)$; $f = 1$

$(dE/dx)_{\text{effective}} = F_D(0) = \alpha\, (dE/dx)_{\text{nuclear}}$

Electronic Sputtering

$\alpha \sim 1\text{-}0.5$ (forward e^-); $f \sim 0.2\text{-}0.4$

f related to e-ph coupling

Typically: $\eta = \eta$ (v)

$\eta \sim 0.2$ for "high" v

$\eta \sim 0.5$ for "low" v

R. E. Johnson and J. Schou, *Mat. Fys. Medd. Dan. Vid. Selsk*. **43** (1993) 403.

Track formation

Electronic Excitations

How do the atoms get extra kinetic energy from the electrons and from other atoms?

$A^+ + A^+ \longrightarrow A^+ + A^+ + \Delta E$ (Coulomb Repulsion)

$(AB)^* \longrightarrow A + B + \Delta E$ (Repulsive Decay)

$A^* + \text{lattice} \longrightarrow A^* + \text{lattice} + \Delta E$ (Lattice Relaxation)

$e(\text{hot}) + \text{lattice} \longrightarrow e + \text{lattice} + \Delta E$ (e-Lattice Heating)

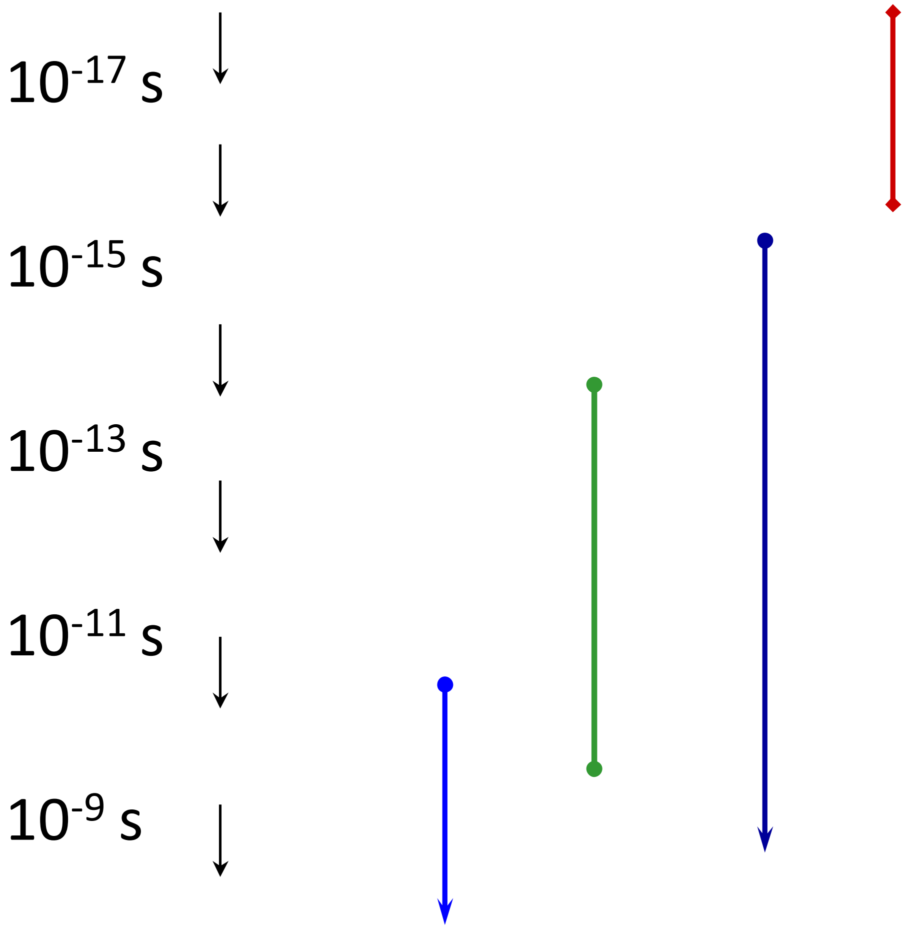
$A^+ + e + e \longrightarrow A^* + e(\text{hot})$ (Dielectronic Recombination)

$A^* + e \longrightarrow A + e(\text{hot}) \longrightarrow A + e + \Delta E$ (De-Excitation)

Other processes…

R. E. Johnson and J. Schou, *Mat. Fys. Medd. Dan. Vid. Selsk*. **43** (1993) 403.

Rough track formation time line



Primary ionizations, excitations and fast delta electrons are produced

Electrons thermalize, decay of excited states, neutralization, hole-hopping.

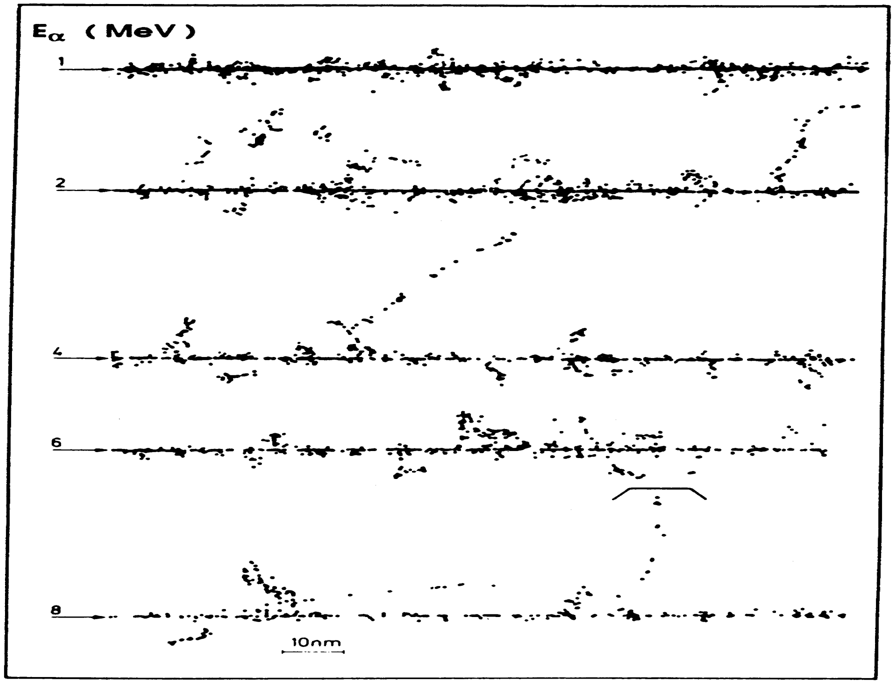
Sputtering, surface modification and defect creation

Luminescence, chemical reactions, defect relaxation

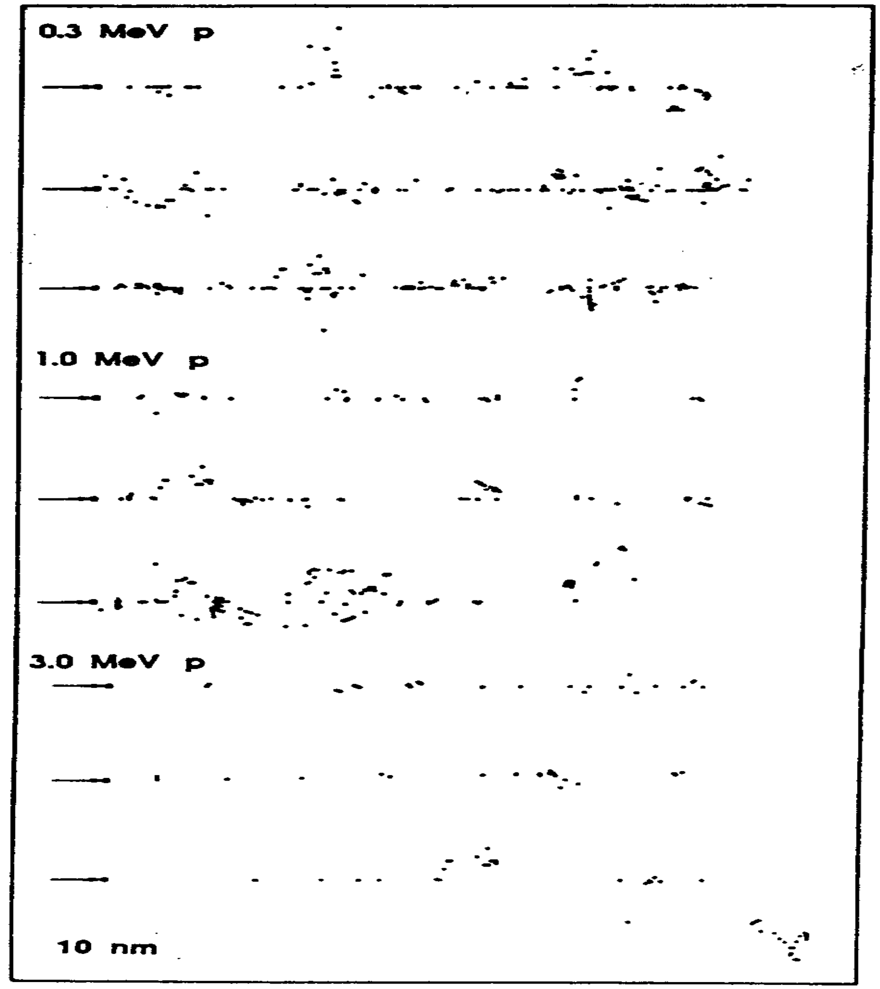
Surface/Bulk defect evolution requires "long" simulations: thermal ejection, recrystalization of simulated amorphous tracks, etc.

R. E. Johnson and J. Schou, *Mat. Fys. Medd. Dan. Vid. Selsk*. **43** (1993) 403.

Tracks in water (MC simulations of ionization)



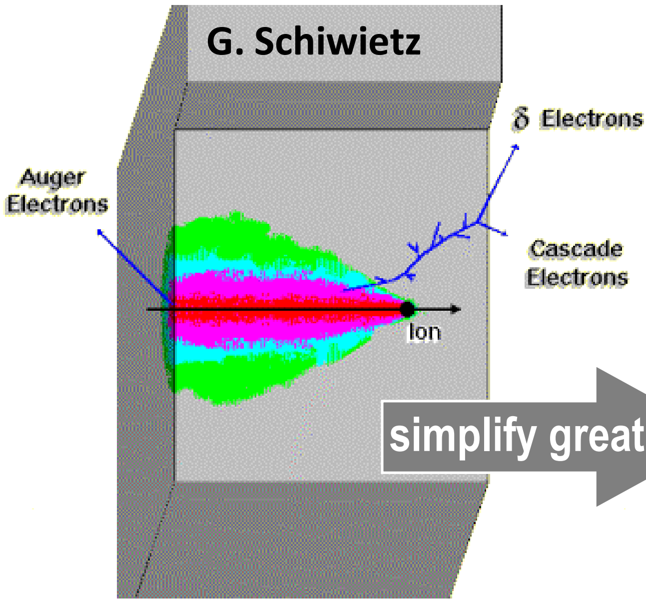
α particles



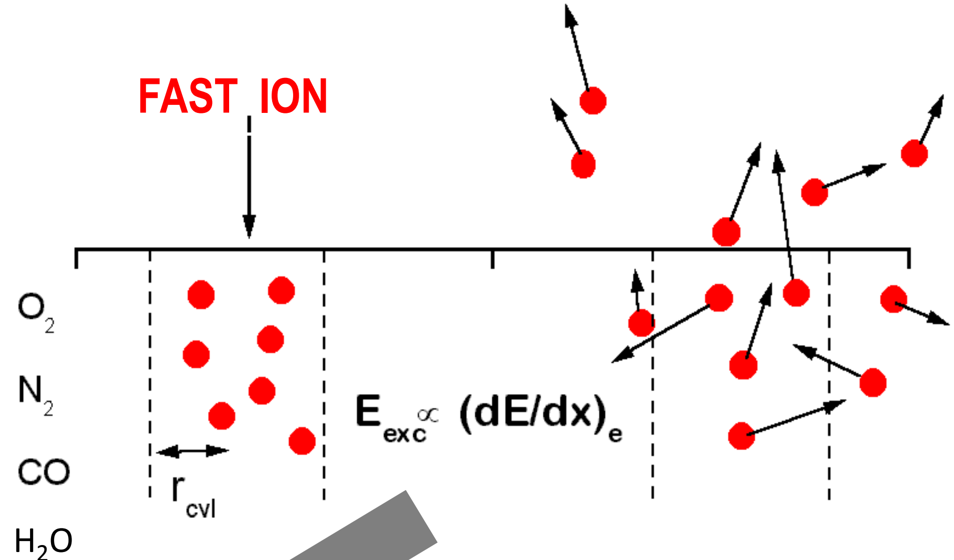
Protons

IAEA-TECDOC-799 *Atomic and Molecular data for radiotherapy and radiation research*, IAEA, Vienna, 1995

Track evolution and modeling



simplify greatly



Many "analytic" models

Coulomb Explosion (few flavors)

Thermal Spikes (many flavors)

Fleisher, Price and Walker, J. App. Phys. **36**, 3645 (1965)

Trautmann, Klaumunzer and Trinkaus, Phys. Rev. Lett. **85**, 3648 (2000)

MORE ....

but MD is often better

MD simulations can predict experimental track sizes

[Devanatham *et al*., NIMB (2008)]

and sputtering

[Bringa and Johnson, PRL **88**, 165501, (2002)]

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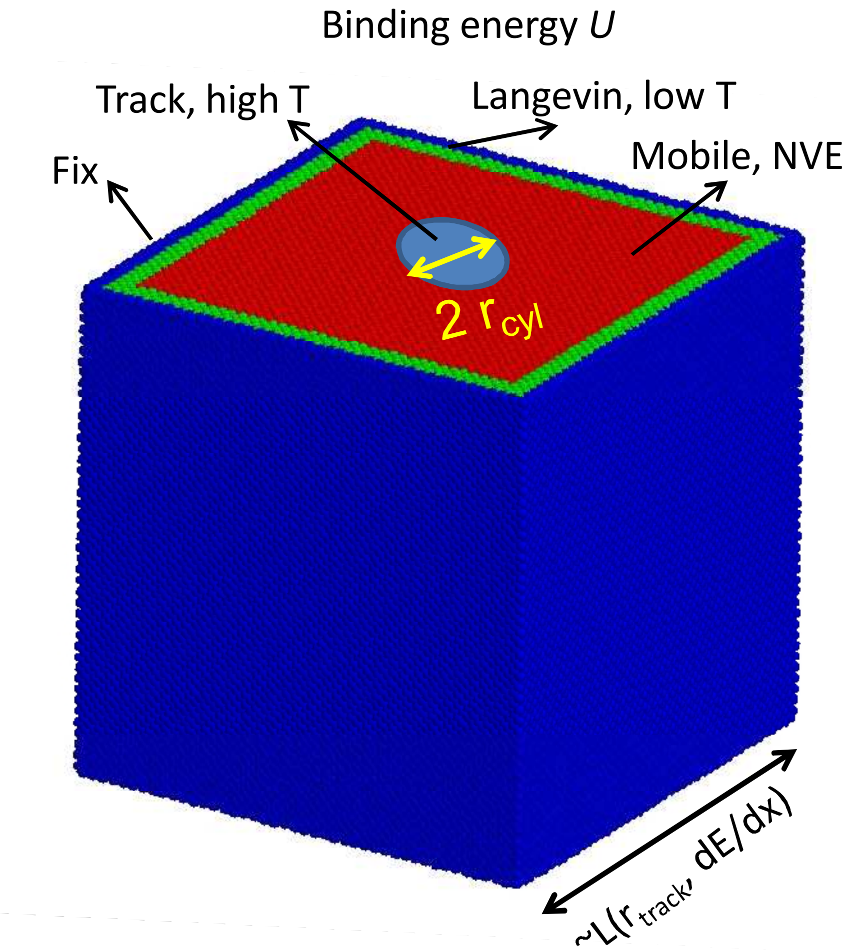
MD Simulations of electronic damage

- Atomic Solid/Molecular solids
  Potentials: L-J, Morse, EAM, oxides, etc. U~0.1-10 eV
- Track: all/few atoms within a region with "radial" symmetry. Cylinder, Gaussian, etc. Size r_{cyl}
- Atoms in track can receive:
  -extra KE (prompt or ramped spike, or from TTM);
  compare with binding energy U;
  -extra charge Z (Coulomb explosion);
  -repulsive or
  anti-bonding potential.



dE/dx ="effective" dE/dx < $(dE/dx)_{exp}$

$R_{cyl} = R_{track}$ (v, dE/dx,etc.)

Variable time step + short-range potentials needed

MD simulation of electronic damage -II

- "Low" *dE/dx* simulations can be carried out with a "diluted" track.
- Velocity effect (i.e. a track size that differs for the same *dE/dx* and different velocity) can be taken into account with different $(dE/dx)_{eff}$ or r_{cyl}.
- For multi-component materials (polymers, alloys, oxides, water, etc.), it can use mass dependent velocity distributions.
- If main excitation decay channel is known, then it can be used instead of simple temperature distribution.
- Can add role of collision cascades, which would be important below/near tracking threshold, by adding a few recoils.
- Charge-state of projectile could be included using different $(dE/dx)_{eff}$.

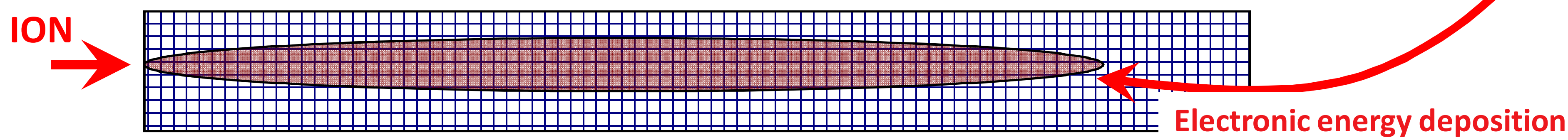
MD track simulations offer a simple empirical way to incrementally add physical information, testing the relative importance of different contributing factors. They help understanding and possible guiding complex experiments, and building larger-scale models.

Combined Two Temperature Model (TTM) – MD

Analytical TTM from 1950s (Kaganov,Lifshits and Tantarov)

$$\begin{cases} C_e(T_e)\dfrac{\partial T_e}{\partial t} = \dfrac{\partial}{\partial z}\left(K_e(T_e)\dfrac{\partial}{\partial z}T_e\right) - G(T_e - T_l) + S(z,t) \\ \cancel{C_l\dfrac{\partial T_l}{\partial t} = \dfrac{\partial}{\partial z}\left(K_l\dfrac{\partial}{\partial z}T_l\right)} + G(T_e - T_l) \quad \Longrightarrow \textbf{MD} \end{cases}$$

$$\text{MD} \quad : \quad m_i\frac{d^2\vec{r}_i}{dt^2} = \vec{F}_i + \xi m_i\frac{d\vec{r}_i^{\,T}}{dt} \quad \text{with } \xi = G(T_e - T_l)\Big/\sum_i\frac{\left|\vec{p}_i^{\,T}\right|^2}{m_i}$$

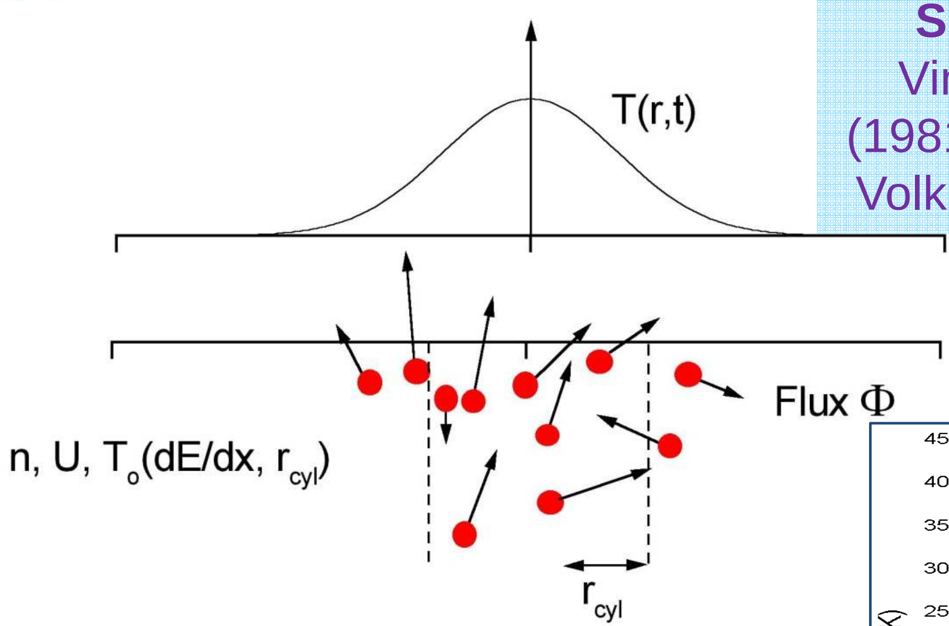


- Toulemonde *et al*. (1994-2011): “Thermal spike” where heating is provided by secondary electrons → spike radius large and E/atom low ➔ neglecting pressure effects is OK.
- TTM (no MD ➔ no pressure/surface) ➔ successful to understand track size data; problems with sputtering data ➔ use more accurate MD+TTM
- MD+TTM first applied to lasers (Zhigilei, Ivanov, Urbassek, 2003), later applied to radiation damage (Duffy, Toulemonde, Nordlund, etc.): S(z,t) ➔ S(r,t) o S(r,z,t)

Analytic Thermal Spike (TS) Models

Semi-analytic models by several groups: Vineyard (1976), Johnson (1980), Sigmund (1981), Toulemonde (1994), Trinkaus, Ryazanov, Volkov, Klaumünzer (1995), Szenes (1996), etc.

Temperature profiles may be used for defect production (tracking), chemistry, etc



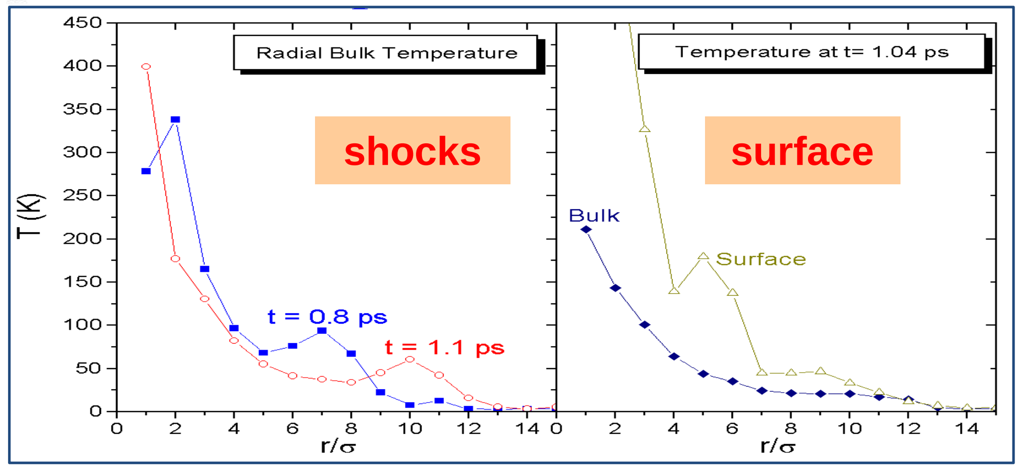
$$Y = \int\int \Phi[T_{surf}(r,t)]\, dA\, dt$$

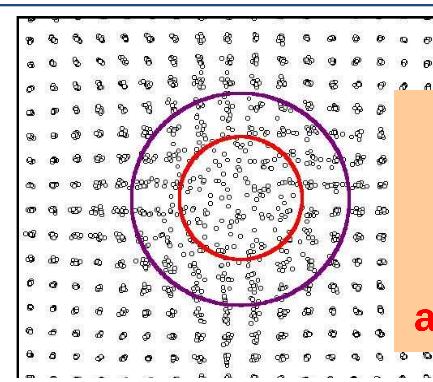
$$Y \propto (dE/dx)^2$$

$$\Phi \propto \exp(-U / k_b T_{surf})$$

$$C(\partial T/\partial t) = \nabla(K \nabla T) \Rightarrow T(r,t)$$

$$T_{surf}(r,t) \sim T(r,t)$$





Molten track does not guarantee "long-time" amorphization

Hydrodynamic Equations for a Thermal Spike also include mass and momentum effects

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$$NC_V\partial T/\partial t = (1/r)\,\partial(rK_T T)/\partial r - T(\partial p/\partial T)N\,\partial v/\partial r + \text{visc.}$$

$$\partial v/\partial t = (1/NM)\,\partial p/\partial r$$

$$\partial N/\partial t = -\,\partial(Nv)/\partial r$$

M = atomic mass, *N* = density

Jakas *et al*., several papers

Alternative to TS: "shock models" which neglect heat diffusion effects

Bitensky & Parillis (1989)

Fenyö & Johnson (1992)

Lesueur & Dunlop (1993)

Few others …. Details: Ryazanov's talk

Melting

$$C_V = \begin{cases} 6/2\ k_B & ;\ T < T_f \\ 3/2\ k_B & ;\ T_f < T \end{cases}$$

$$C_V \rightarrow C_V + Q_{fus}/10;\quad \text{if}\quad T_{fus} - \Delta T < T < T_{fus} + \Delta T$$

MD: have to be careful with "localized" phase changes and temperature/pressure calculations.

Thermal conductivity

$$K_T = (25\,k_B/32\sigma_0)(\,k_B T/\pi\,M)^{1/2},\quad \sigma_0 = 1.151\ \text{Å}$$

Semi-Analytical Thermal Spike models vs. MD

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•Semi-analytical TS models do NOT give good description of energy transport and sputtering at high energy densities ($E_{exc} > U$).

•MD treats properly energy transport (thermal properties, phase transitions, pressure effects) and **<u>surface</u>**.

•Assumptions about initial energy deposition are needed to understand experiments: electron-phonon coupling or effective *dE/dx*, initial track radius, velocity effects, etc.

•**Drawback:** models takes few minutes, MD takes few days ☺

First large-scale MD simulations of Coulomb Explosion (induced by slow-Highly Charged Ions)

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Hai-Ping Cheng and J. D. Gillaspy, PRB **55** (1997) 2628

Initial simulations of HCI had no neutralization

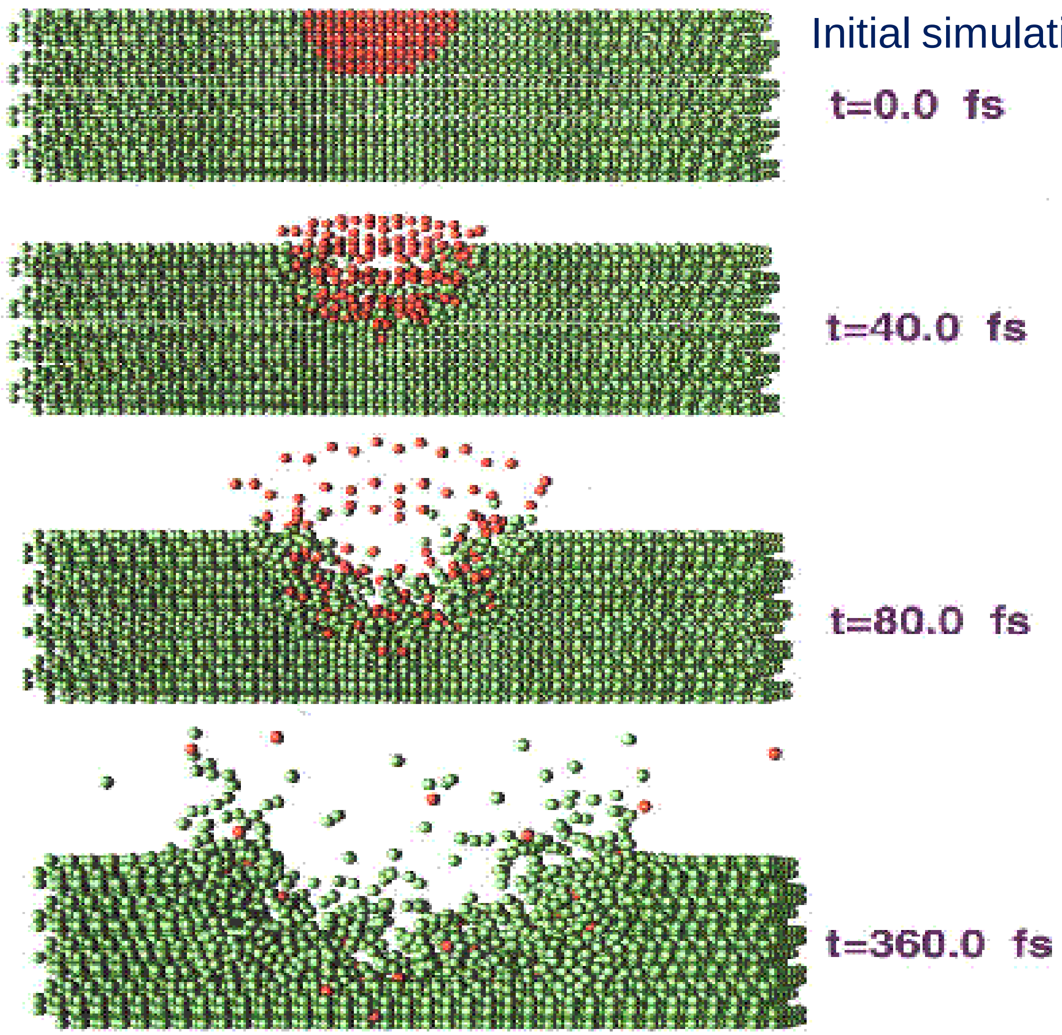
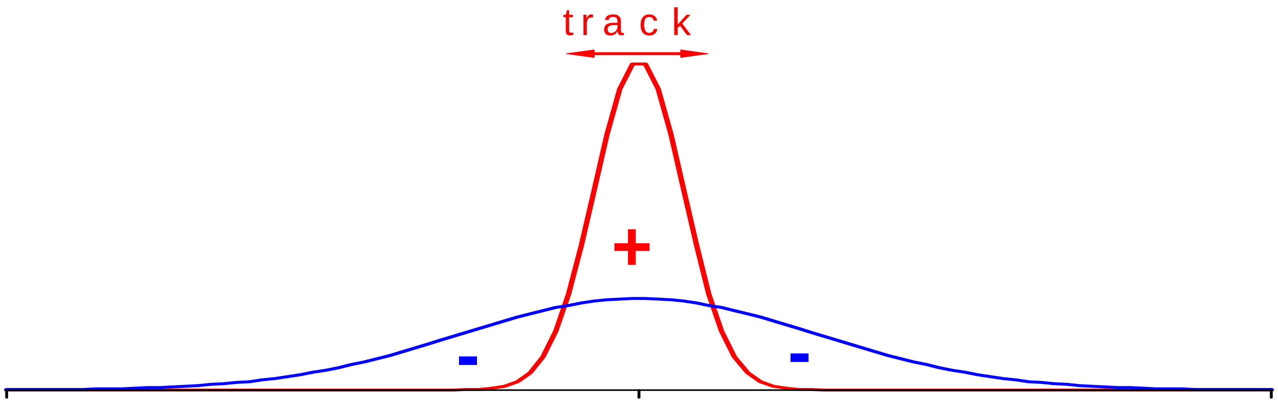


FIG. 1. (Color) Snapshot of the time evolution of the Coulomb explosion process. Red and green spheres are used to indicate Si^{m+} ions and Si atoms, respectively. This particular system consists of 365 ions. The initial Coulomb repulsive energy stored in the hemispherical region is about 87.3 keV. Between $t=0$ and 40 fs, the charged region expands significantly. At $t=80$ fs, over 100 ions are ejected from the surface, forming a pronounced hole. By 360 fs, the hole is much larger, and about 800 atoms and ions are driven from the surface.

Many semi-analytical models of CE (Ryazanov's talk).

Several other previous simulations of CE, including CE in ionic crystals [Walkup & Avouris, Phys. Rev. Lett. (1986)].

Simplified view of screening



"Free" electrons screen the ions in the track

"Static" screening: $V(r) = (Ze)^2 \, Exp(-r/a) / r$

Classical plasma

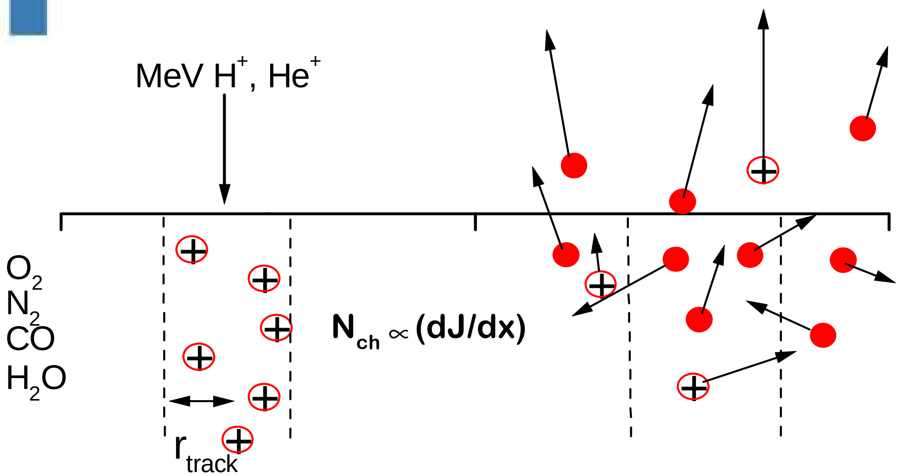
$a = v_T/\omega_p$ Debye screening

Quantum plasma

$a \sim v_F/\omega_p$ Thomas-Fermi screening

Use MC modeling with electron cross-sections/mean free paths to estimate time dependent screening

Coulomb explosion (CE) simulations



$$PE \sim (N_{ch}e)^2/d \longrightarrow \Delta KE$$

$$Y \propto (dJ/dx)^2$$

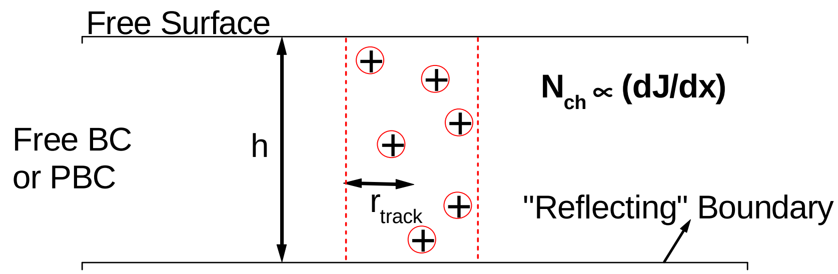
$$dJ/dx = A\,(Z_{eff}/v)^2 \ln(B\,v^2) \propto (dE/dx)_e$$

- Extremely difficult to determine neutralization times, both theoretically and experimentally
- If net repulsion is due to excited states, they may decay too fast, or they may diffuse far away before decaying.

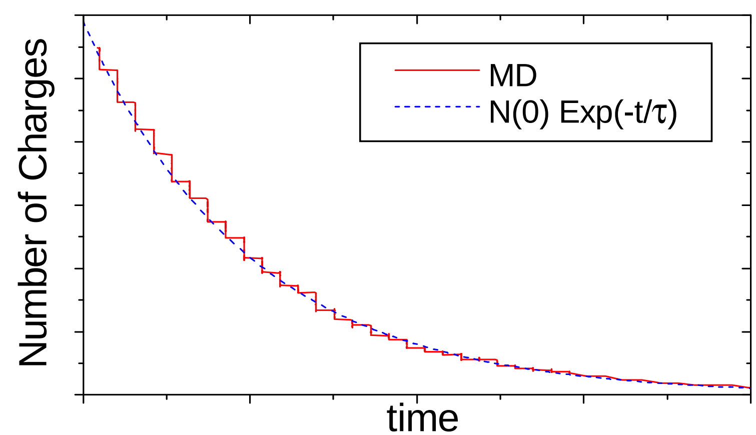
MD Simulations of Coulomb Explosion

$V(r_{ij})=V_{L-J}(r_{ij})+(Z_iZ_j/r_{ij})\,\mathrm{Exp}(-r_{ij}/a)$. $r_{cut\text{-}Coul}= 7\,a$

depth of layer $h > 2\, r_{cut\text{-}Coul}$. r_{track} / $N_{ch\text{-}MAX}$= 2 charges/layer



Neutralization Time τ



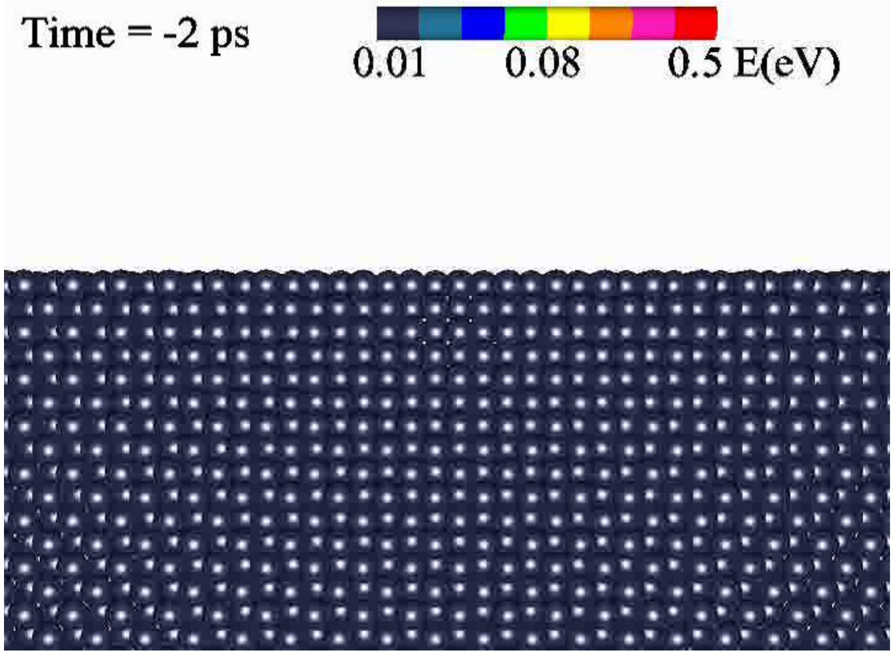
Bringa and Johnson, PRL **88**, 165501 (2002)

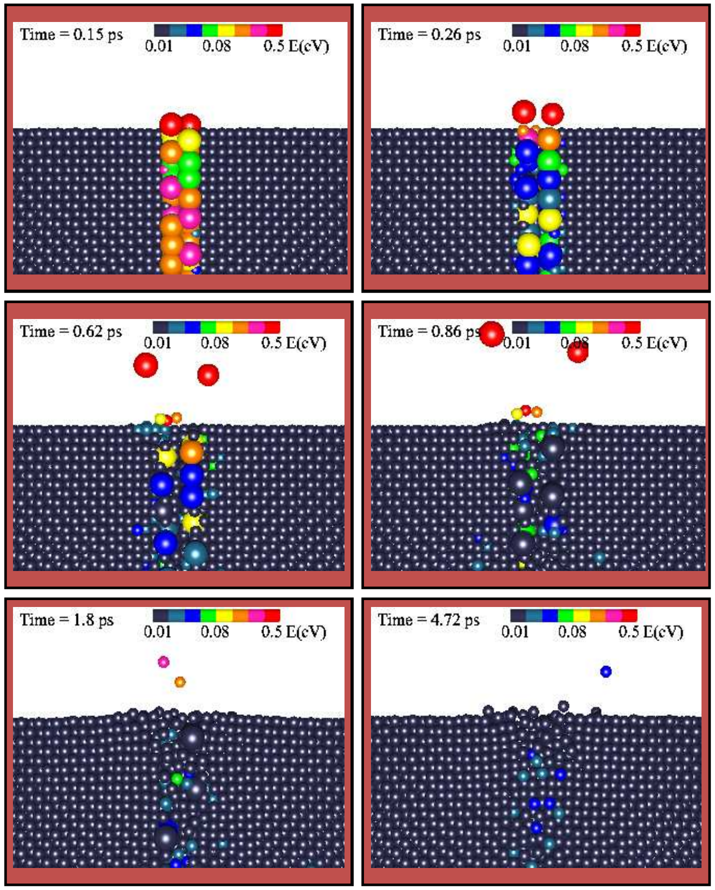
Similar to H-P. Cheng work for HCl

Coulomb Explosion MD simulations

N_{ch}=2, $a \sim l$, $r_{track} \sim l$, τ=1 ps~2 t_D

charged atoms have twice the radius of neutral atoms

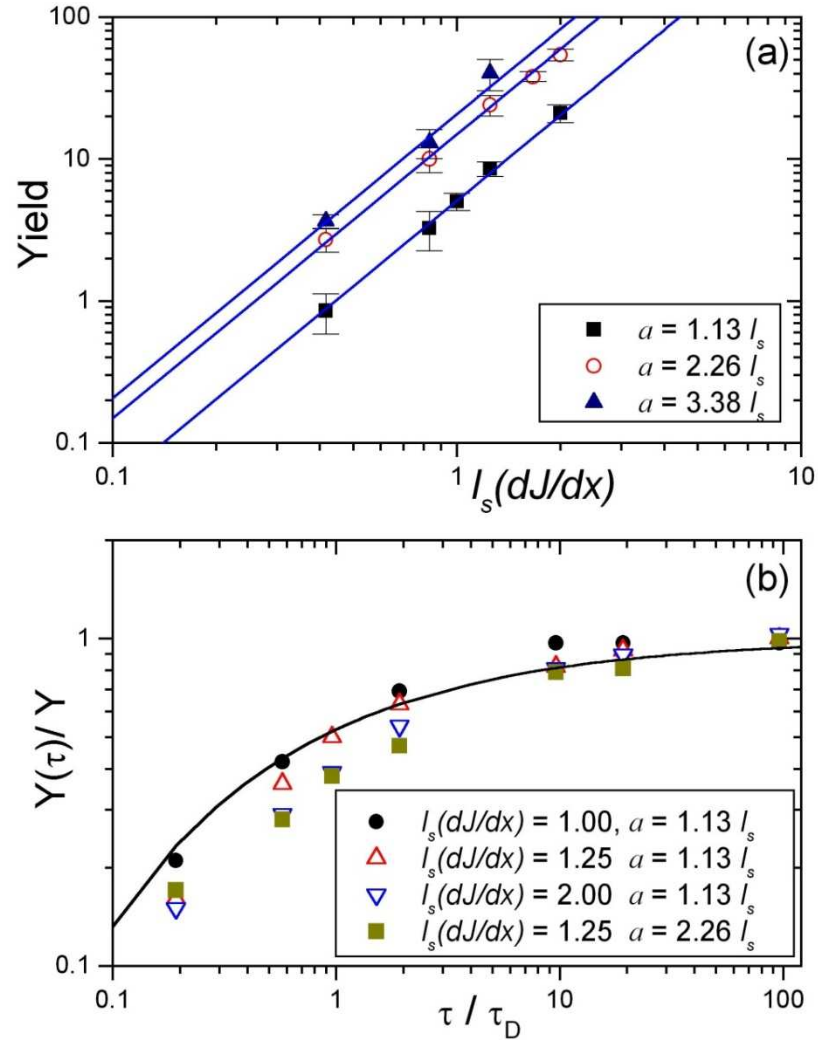




If neutralization is too fast there is no heating of the lattice!

Bringa, NIMB (2002)

Coulomb explosion leads to heating of the lattice as in TS



$Y \sim (dJ/dx)^2\, ln(a)$

Bringa and Johnson, PRL **88**, 165501 (2002)

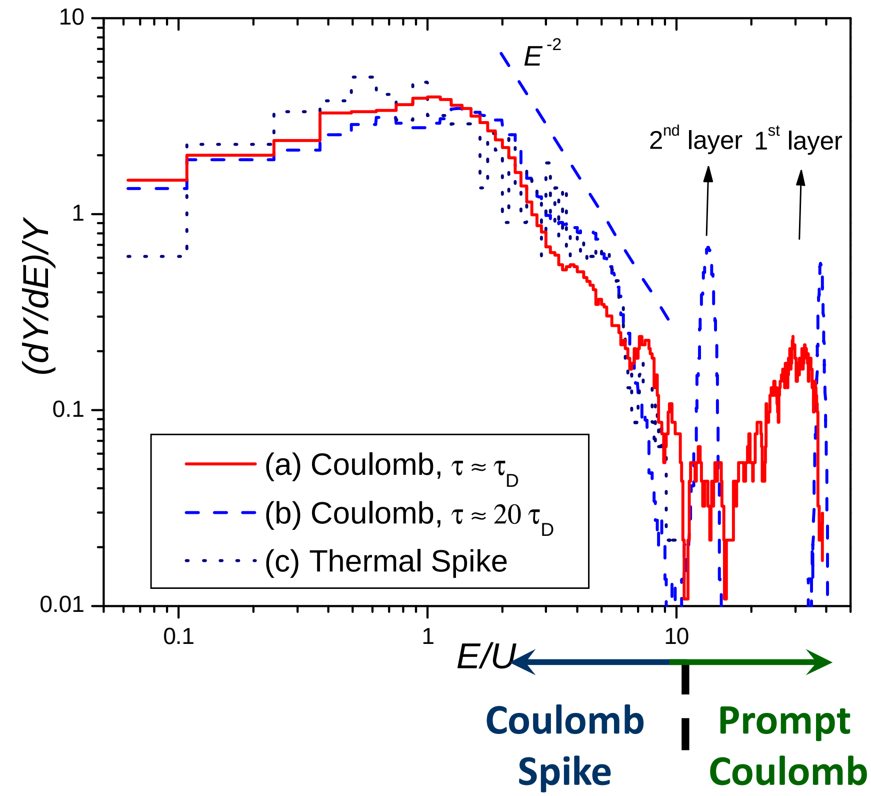
Is there a thermal spike (TS)? YES!

Analyzing MD data, there is a clearly defined energetic track with:

1) $(dE/dx)_{eff} = A\,(dJ/dx)^2$

2) r_{cyl}= *Constant*

$\Rightarrow$ $Y_{MD\text{-}CE} = Y_{MD\text{-}TS}$



Old idea: "Thermalized" ion explosion model

L. E. Seiberling, J. E. Griffith, and T. A.Tombrello, Rad. Eff. **52** (1980) 201

Ryazanov *et al*. have similar model, including coupling to MD

- Coulomb explosion heats up the atoms at the track.
- Sputtering as in the thermal spike model.

$Y \sim \Delta A \Delta t\ \mathrm{flux}(T) \sim \pi r_{cyl}^2 (r_{cyl}^2/4K)\ \mathrm{flux}(T)$

$Y \sim (dJ/dx)^4$, $Y \sim (dJ/dx)\exp[-U r_{cyl}^2/(dJ/dx)^2]$

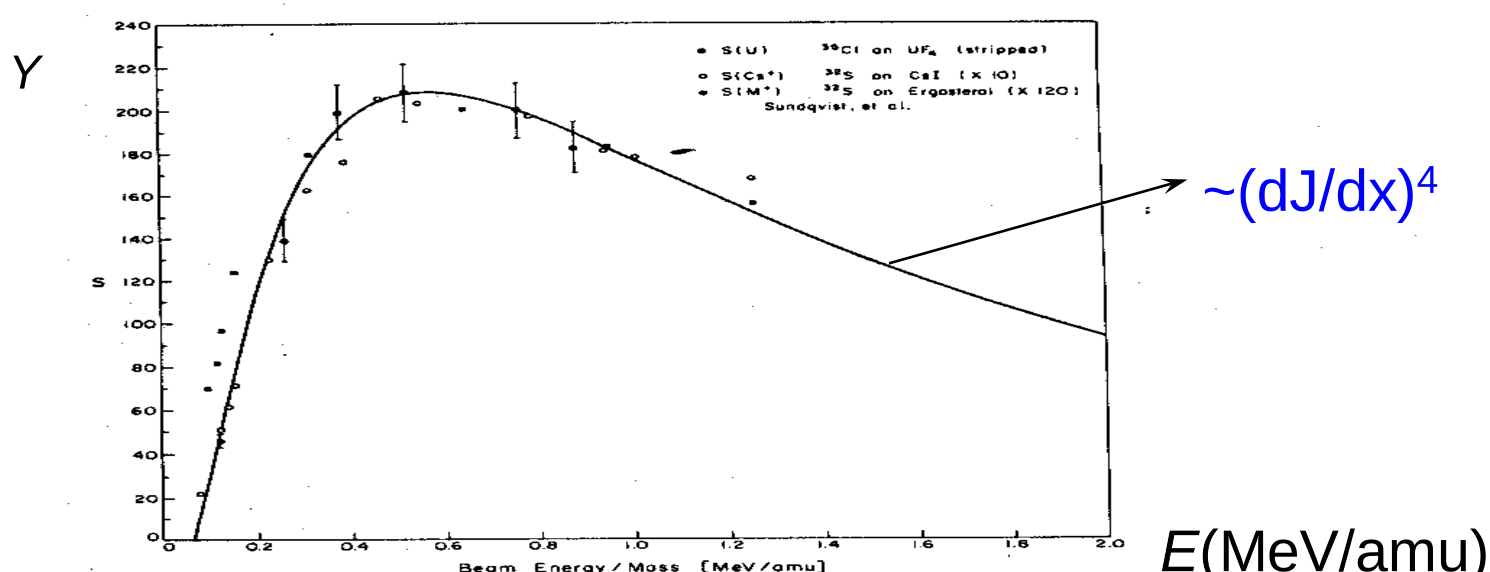


Fig. 4. Sputtering yield data versus beam energy per atomic mass unit for chlorine ions incident on UF_4 from a "stripped" experiment. Also shown are sputtered ion yields for sulfur ions on CsI and ergosterol targets (23). $S(M^+)$ refers to the sputtering yield of (ergosterol)$^+$ ions. The curve is a fit to $(dJ/dx)^4$ (see text, section 2).

Summary of recent MD simulations of electronic damage

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- Many papers using instantaneous energy deposition in cylindrical track (Urbassek & Johnson 1994, Bringa *et al*., PRL, PRB, NIMB, Surf. Sci, etc. 1996-2011).
- Analytical models OK at low energy density but do not work at high energy density: pressure + surface effects + Non-LTE are a problem (Bringa et al., NIMB + PRB).
- Hydrodynamic model fit to MD works very well (Jakas *et al*., PRB,NIMB,1999-2002).
- Simulation results for sputtering of Lennard-Jones model solid agree with simulations for more complex materials (Bringa *et al*., Surf. Sci. 2000; Tucker *et al*., NIMB 2005).
- Difficult to connect experimental *dE/dx* to energy deposited in simulation (Toulemonde, Tombrello, Szenes, etc., mostly in NIMB and PRB).
- Can use more complex models of track heating, for instance TTM (Toulemonde *et al*., many papers PRB/NIMB).
- Results from Toulemonde, Beuve, and co-workers show variation of results when adding temporal and spatial effects in track heating (PRB, NIMB 2001-2008).
- TS useful for track formation simulations in bulk (Devanathan *et al*.; NIMB 2007, Schwen & Bringa, NIMB 2007; Kluth *et al*. PRL 2008, Duffy, several papers 2006-2010).
- Useful model: cluster-induced nuclear sputtering and damage (Brunelle NIMB 2004).

Two questions …

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Given all the approximations and limitations involved …

- Can we hope for quantitative agreement between MD and experiments when electronic effects are important?

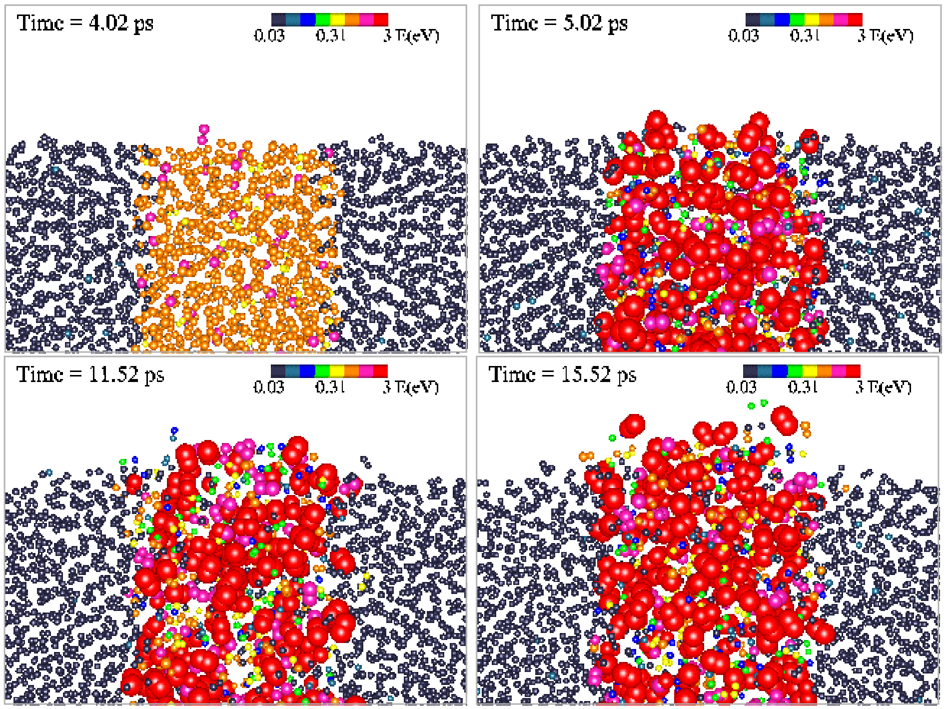
OR …

- Is MD just pretty movies and pictures?

OUTLINE

- Background and Introduction
  - Track models
- Molecular Dynamics (MD) of damage in the electronic regime
  - Thermal Spikes, Two Temperature Models and Coulomb Explosions.
- Examples
  - Electronic sputtering, track formation: defects, phase change, craters & bumps
- Conclusions and future outlook

Example I: Electronic sputtering of solid oxygen

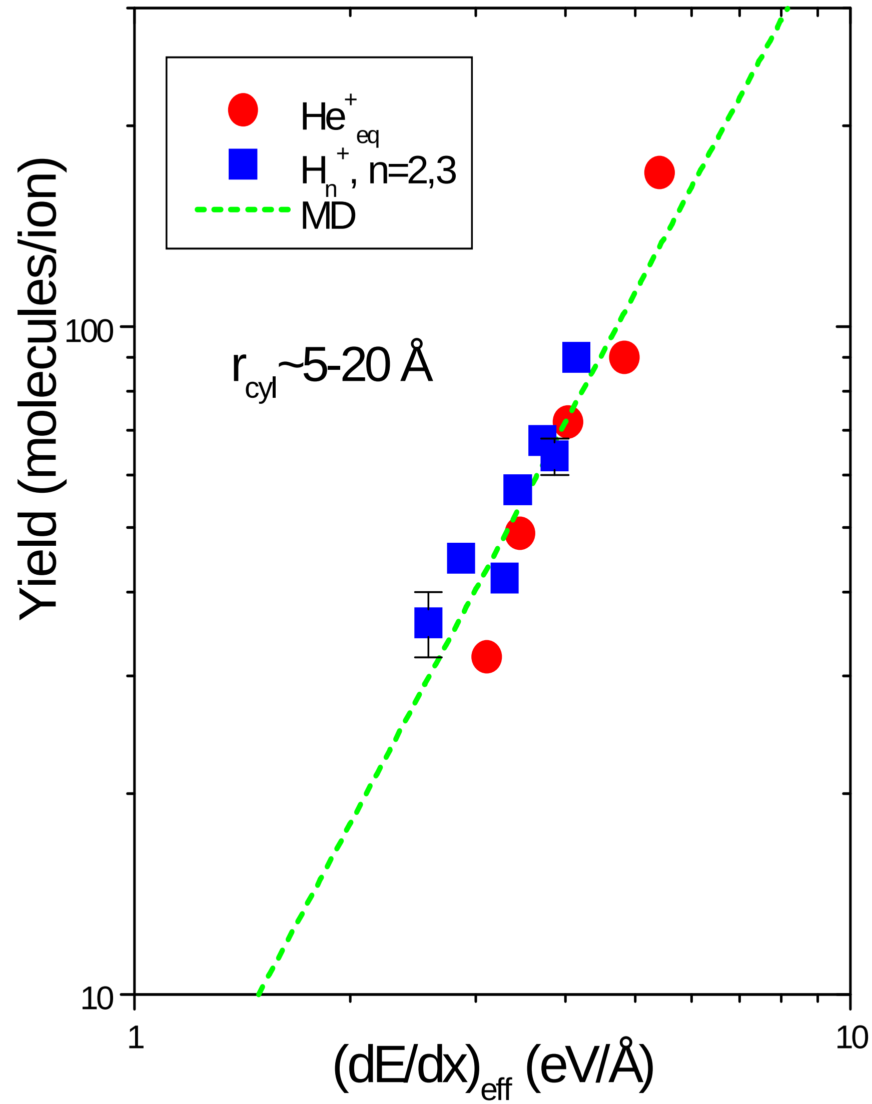


Vibrational Excitation of Solid O_2, side view

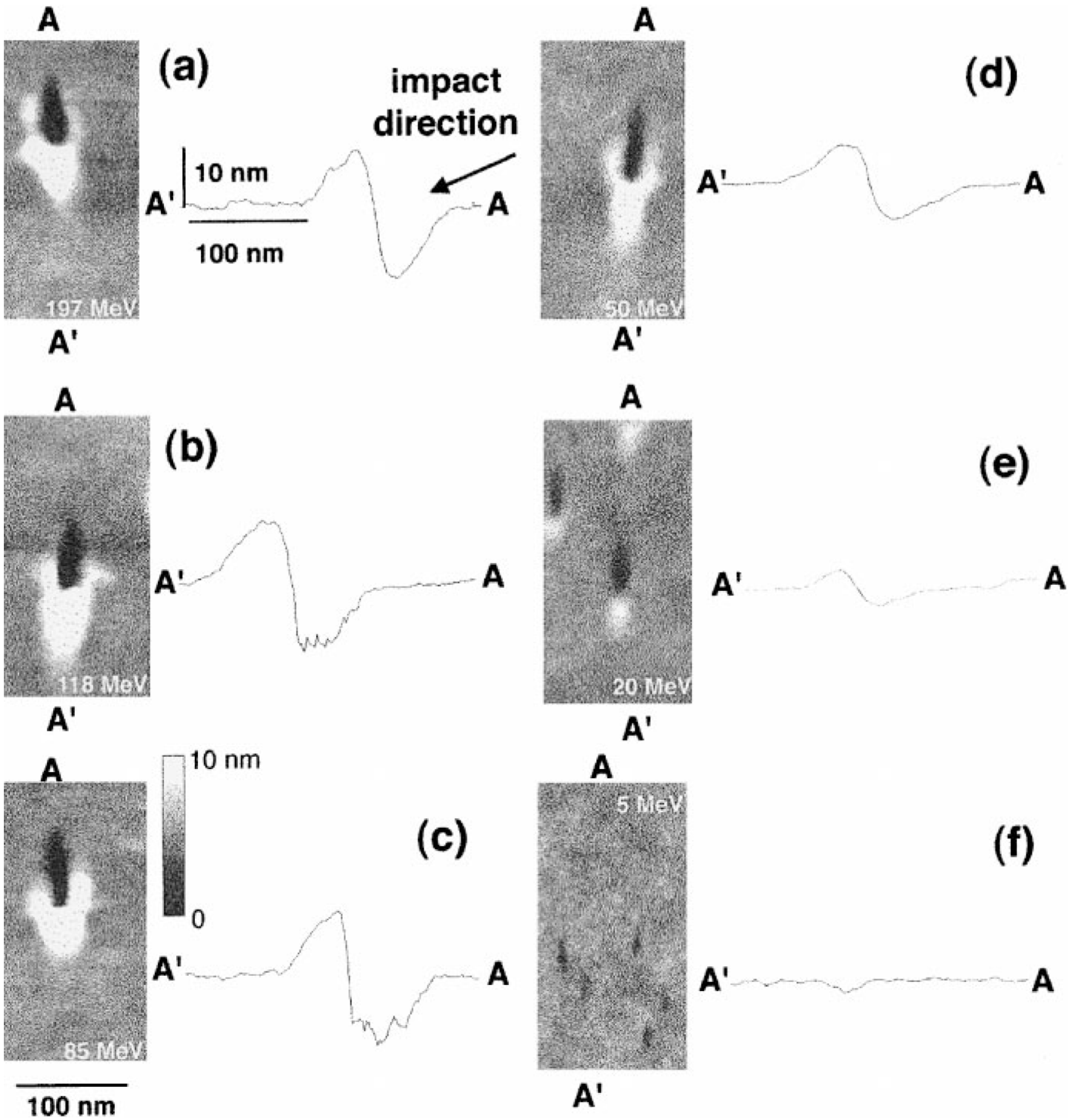
r_{cyl}=6 , E_{exc}=4 eV

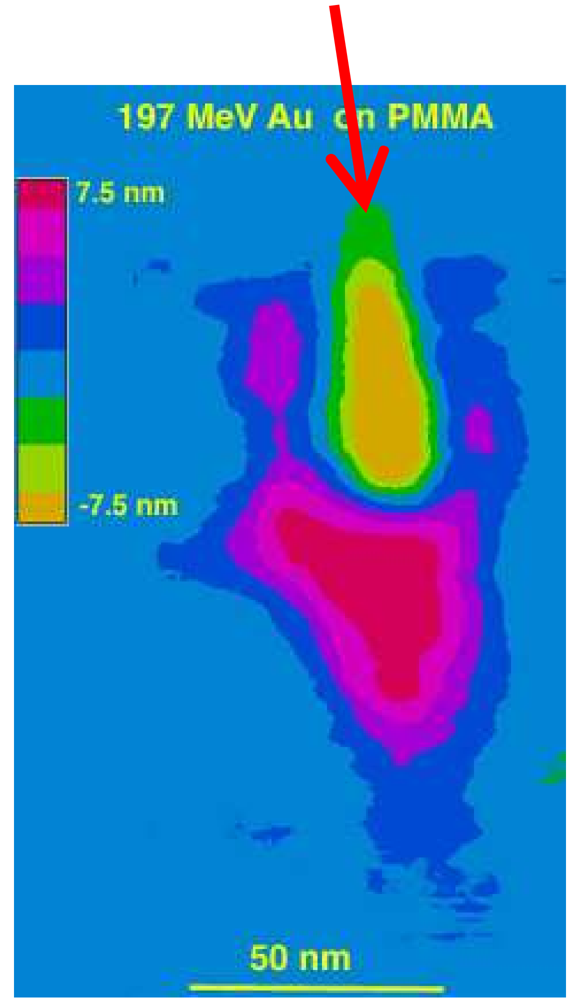
Bringa and Johnson, Surface Science (2000)

Includes "velocity effect" in track size



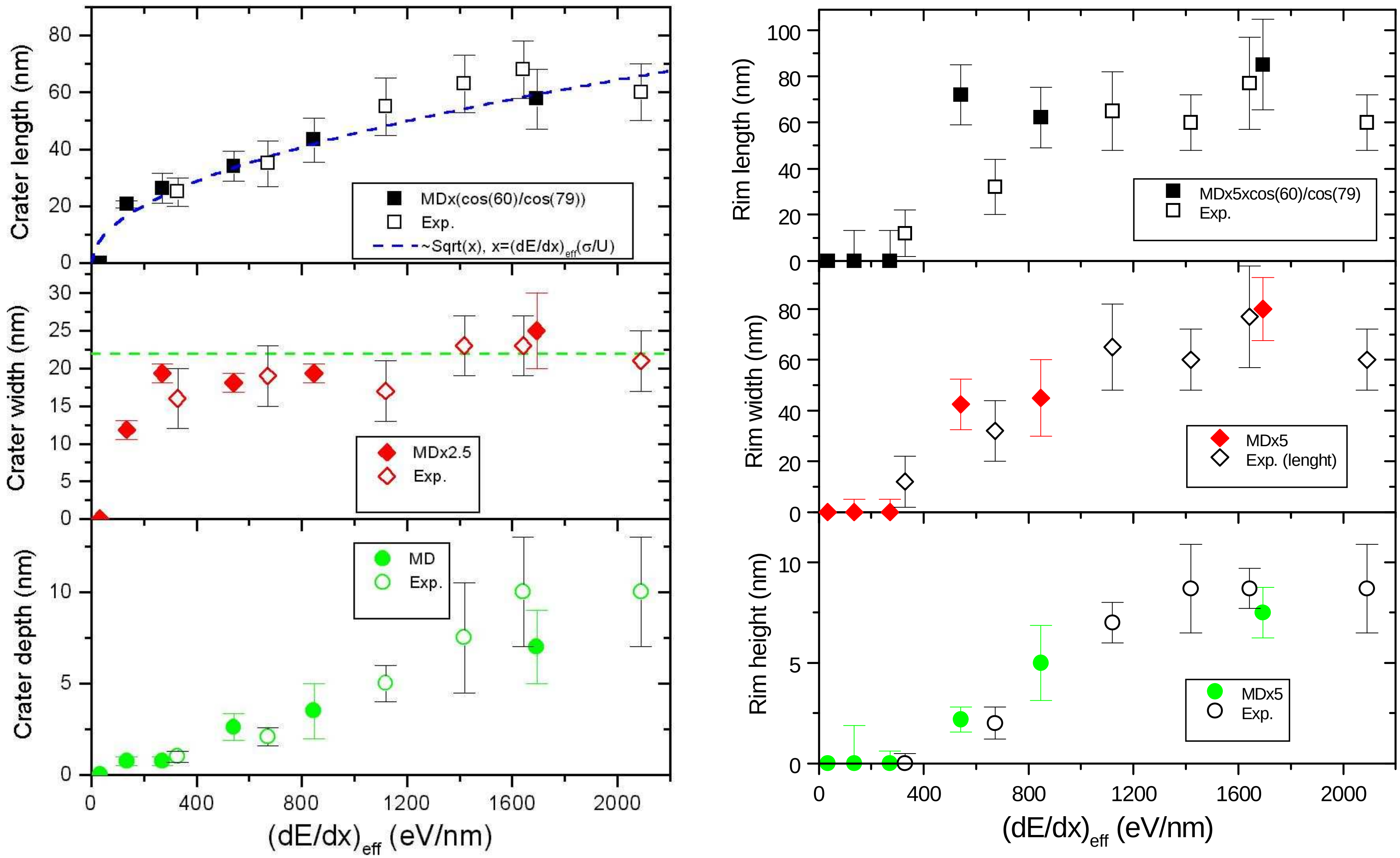
Example II: Cratering in PMMA





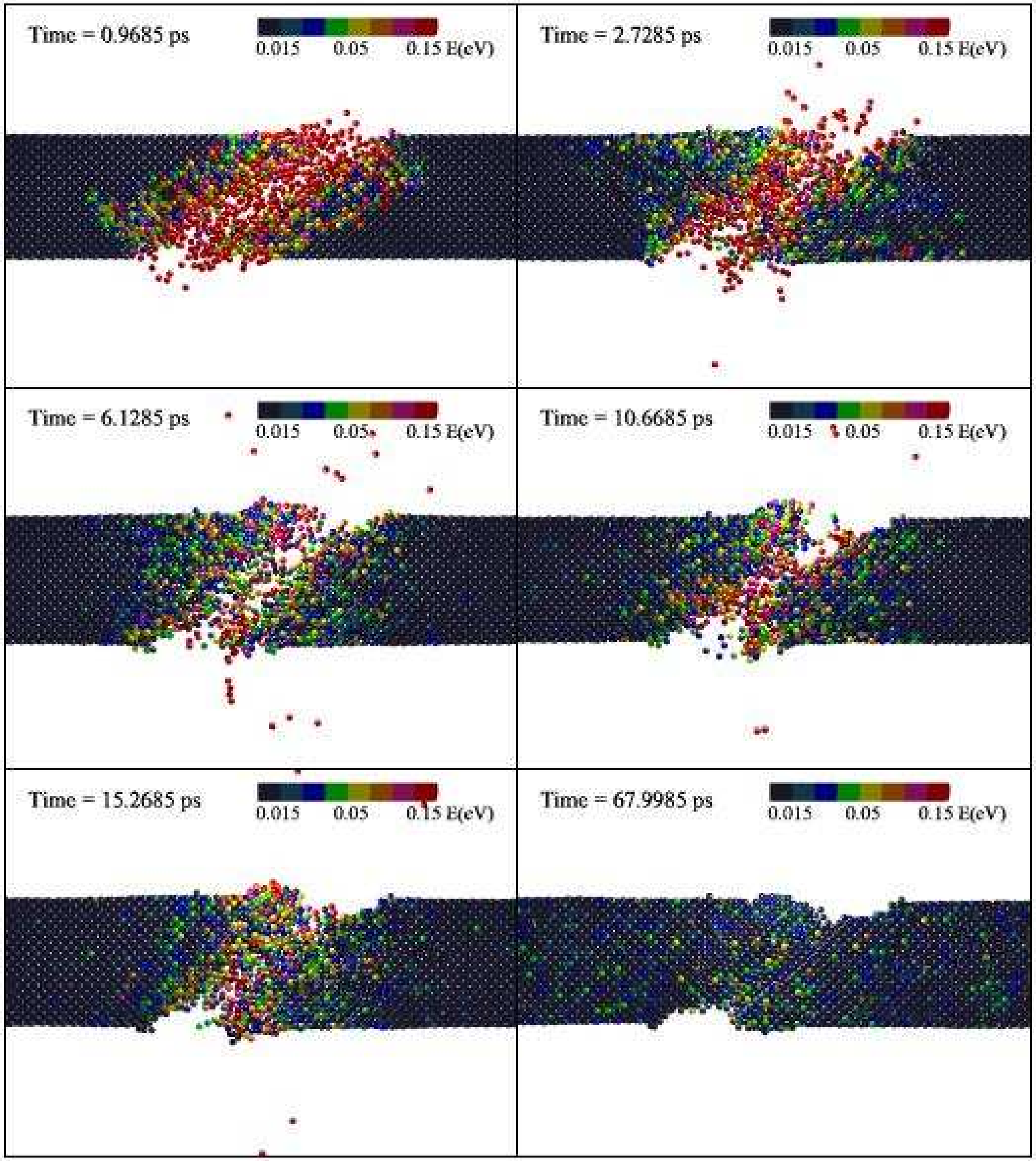
Experiments by R. Papaléo *et al.*
(several papers)

Crater size (R. Papaléo *et al.*) agrees extremely well with MD



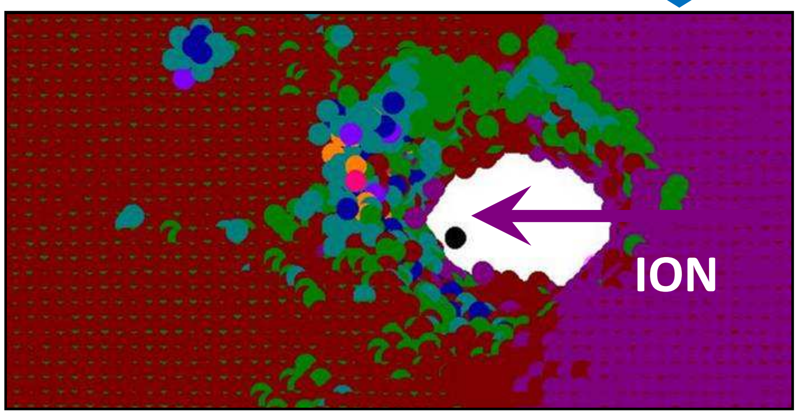
Bringa *et al.*, PRB, NIMB

Example III: Can we create nano-holes? YES



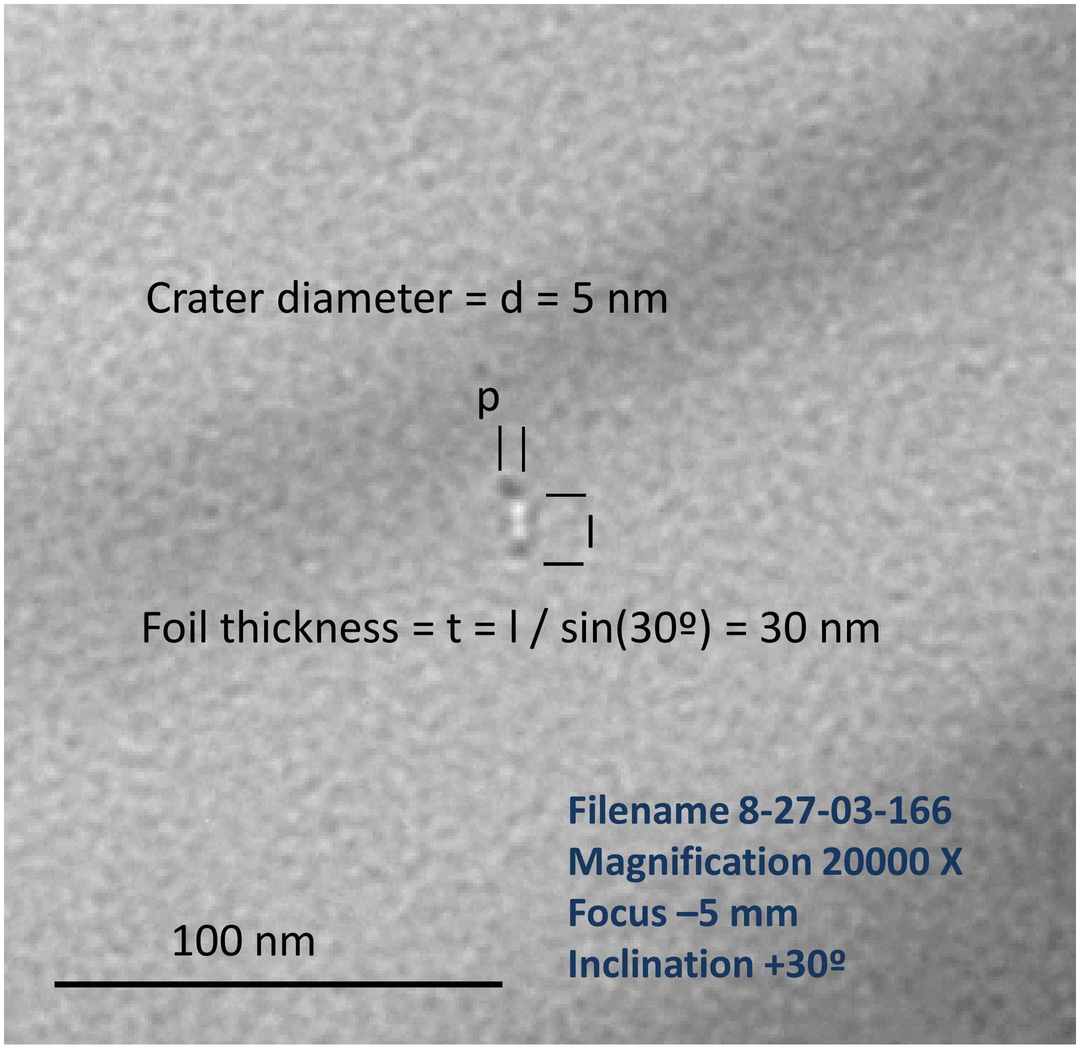
If the thin-film is too thick, the track not wide enough, or the energy deposited not high enough, only a crater is formed (no hole)

4 times more energy in the track (other parameters the same) ➔ hole is formed!
remains stable and cool after 100 ps

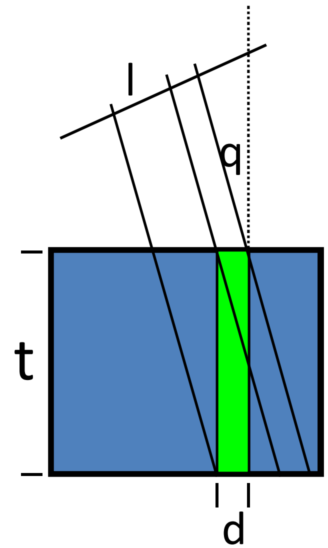


TEM observation of double nano-craters

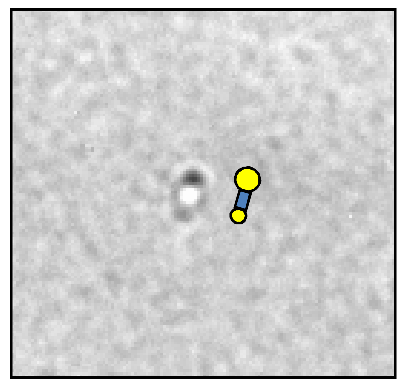
Follstaedt, Rossi and Doyle (SNL): Au (374 MeV) → sapphire



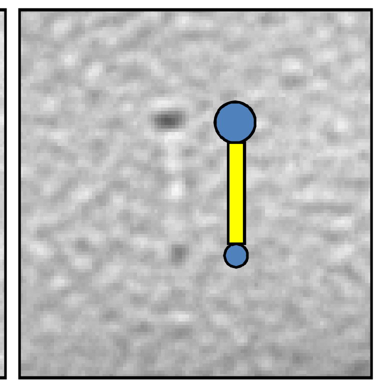
Follstaedt *et al.*, NIMB 2006



θ, angle of view
t, foil thickness
l, TEM 2-craters-distance
d, true crater diameter
p, TEM crater diameter



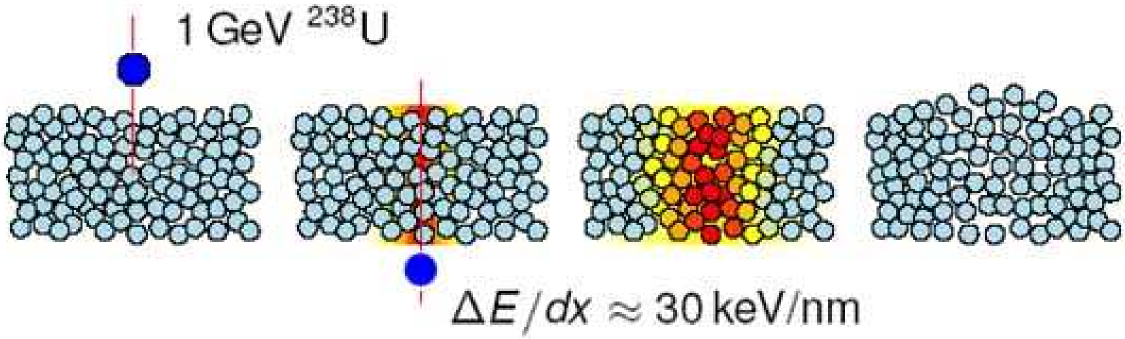
20º

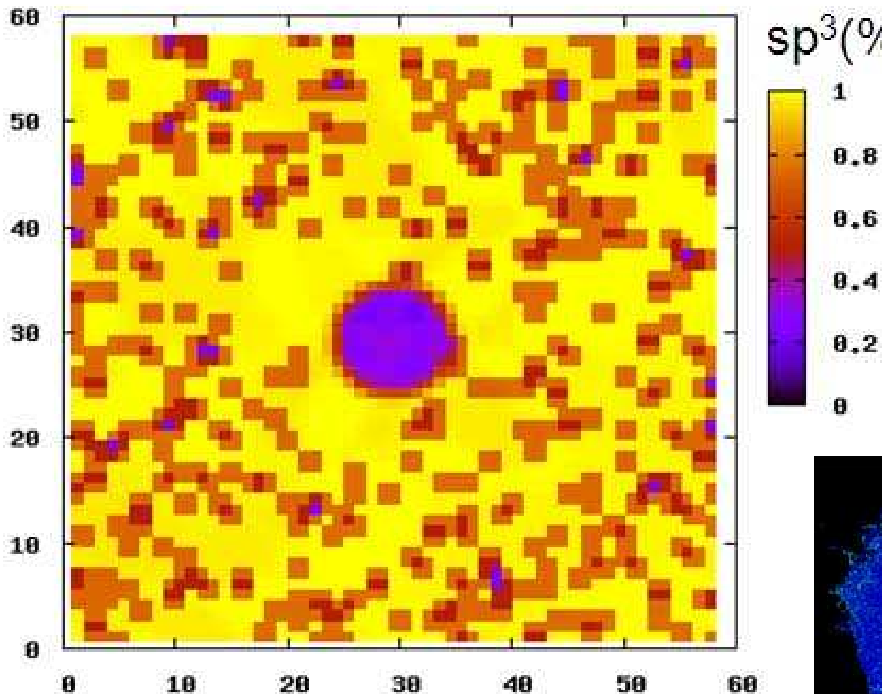


45º

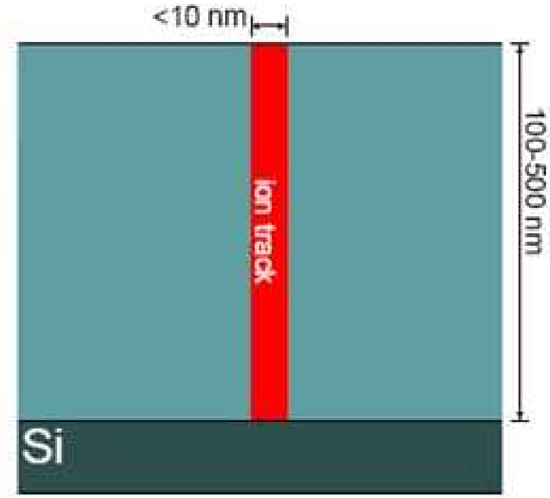
Asymmetry in crater size possibly due to δ e$^-$ asymmetry?

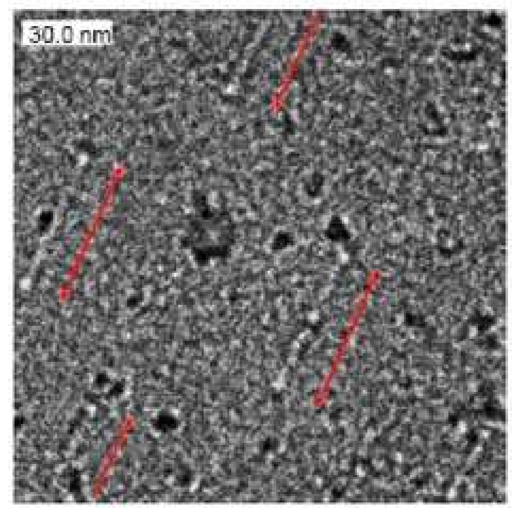
Example IV: Tracks in ta-C create conducting nano-wires

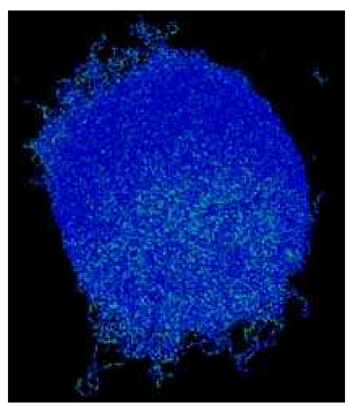




Simulations and experiments display creation of sp^2 rich region



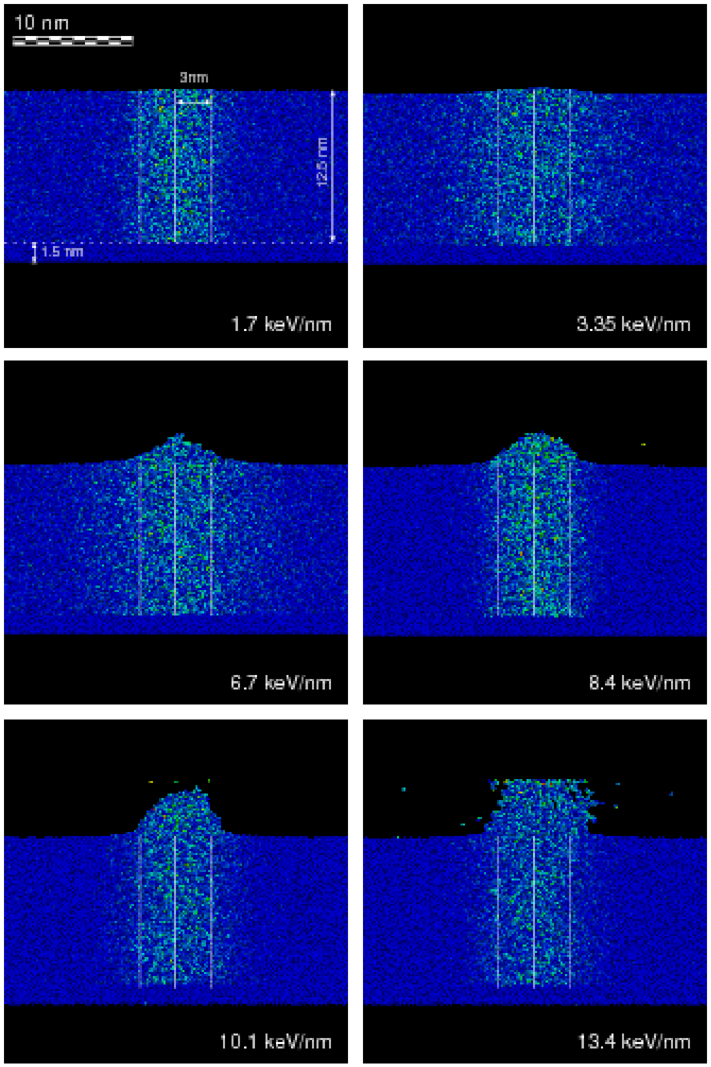


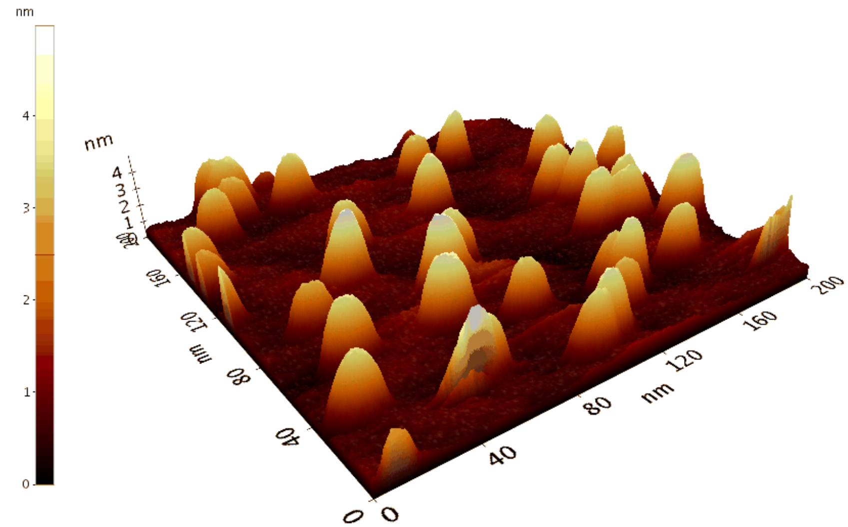


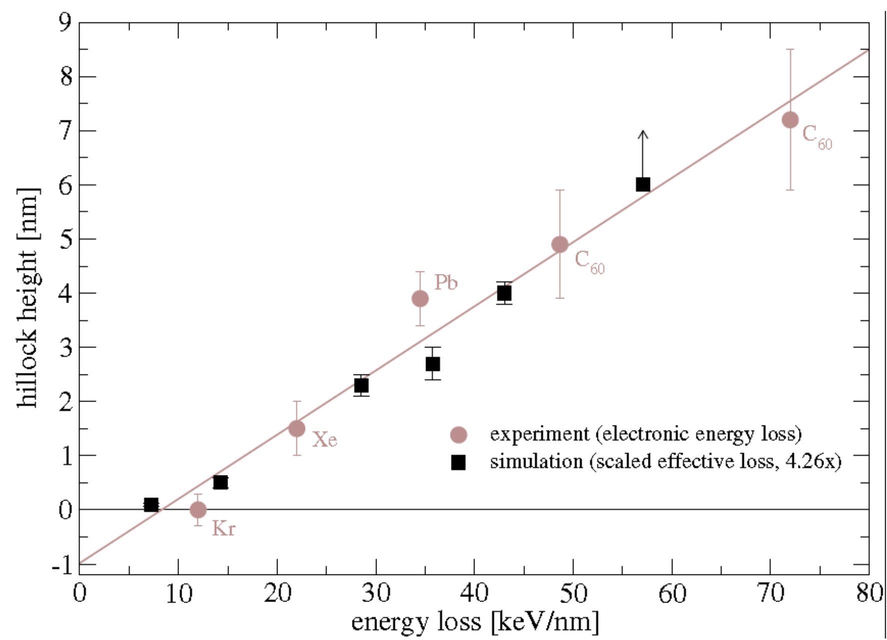
Cosmic ray destroying a carbon grain

Schwen & Bringa, NIMB 2007

Hillock formation (2 10^6 atoms, modified Brenner potential)

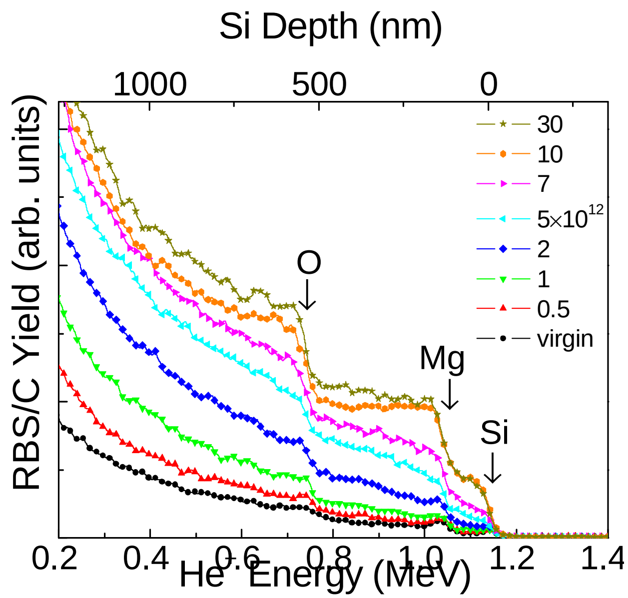




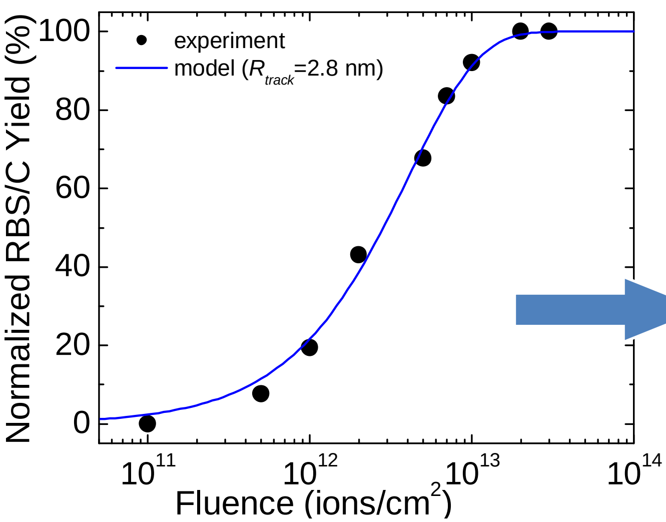


Schwen & Bringa, submitted (2011)

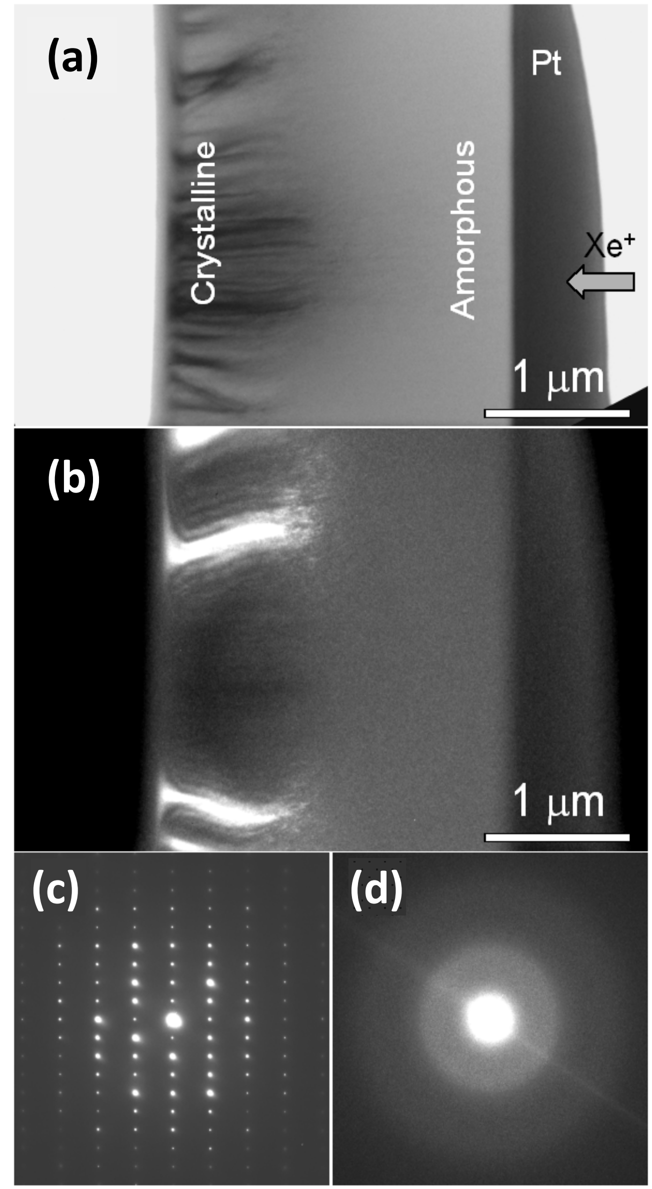
Example V: Amorphization of forsterite (Mg_2SiO_4) by electronic effects



10 MeV Xe bombardment of single crystal forsterite
S. Kucheyev and T. Felter (LLNL)



Amorphization dose calculated from RBS/C, and confirmed by TEM/XRD of irradiated samples



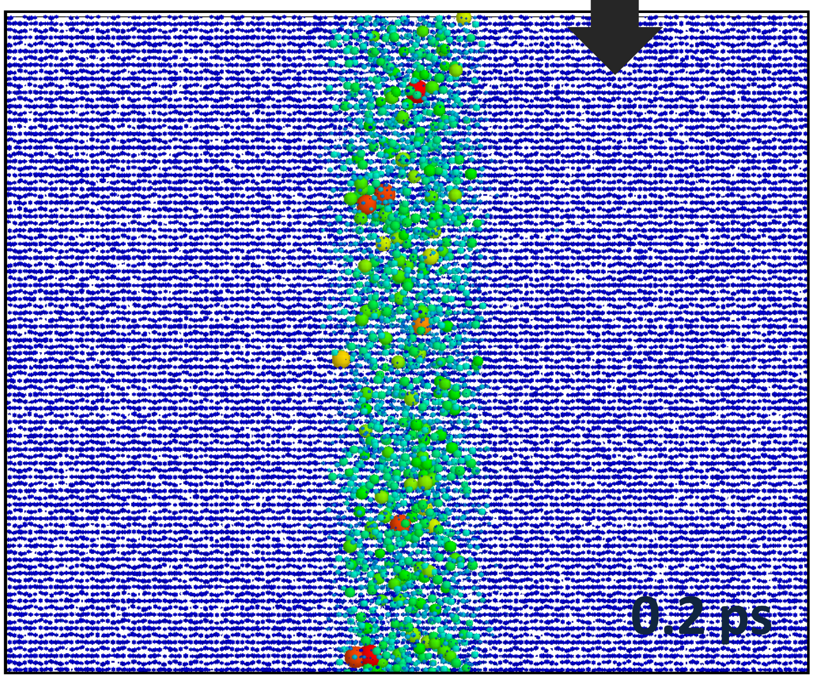
Bringa *et al*., ApJ. (2007)

MD simulations of amorphization

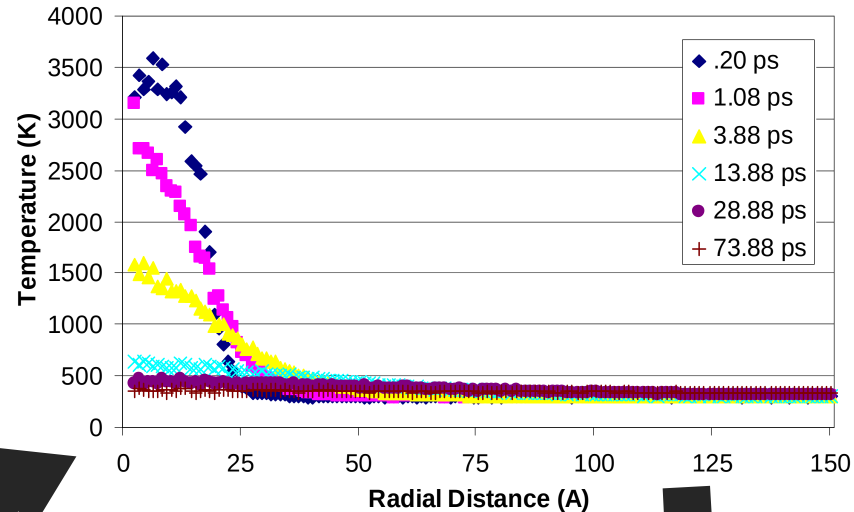
P. Durham (LLNL/Cincinnati), R. Devanatham, R. Corrales (PNNL)

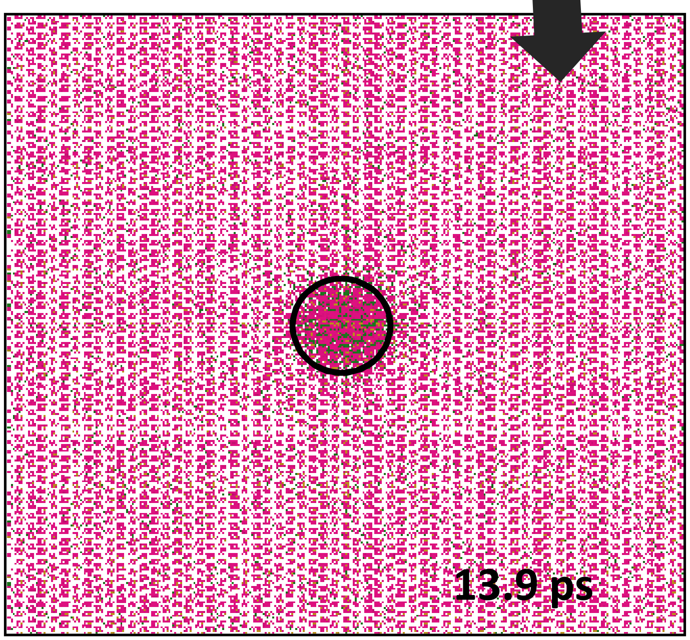
SiMAF

- DL_POLY with parallel domain decomposition, 32-128 CPUs, 10^4-1.25 10^6 atoms.
- Buckingham potential + SPME
- Thermal spike model
- New local order parameter to detect amorphization



Devanatham *et al*., NIMB (2007)

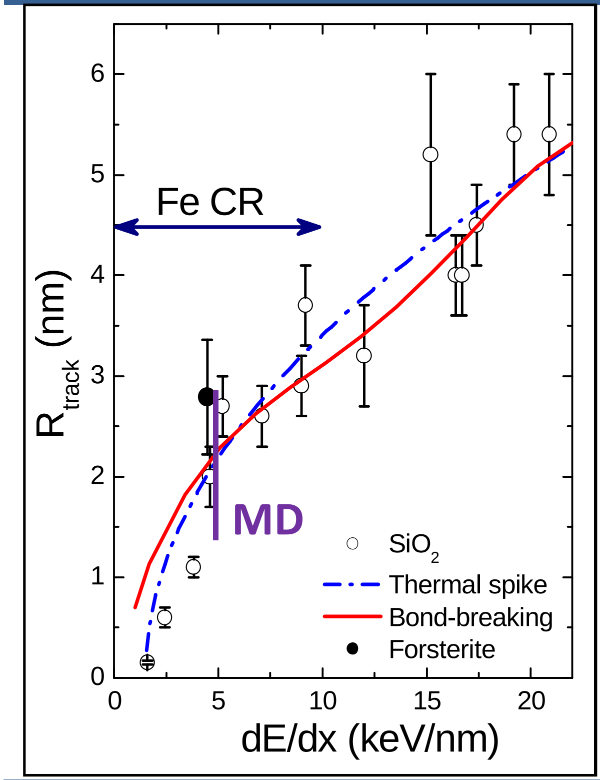




Silicates can be amorphized by cosmic rays

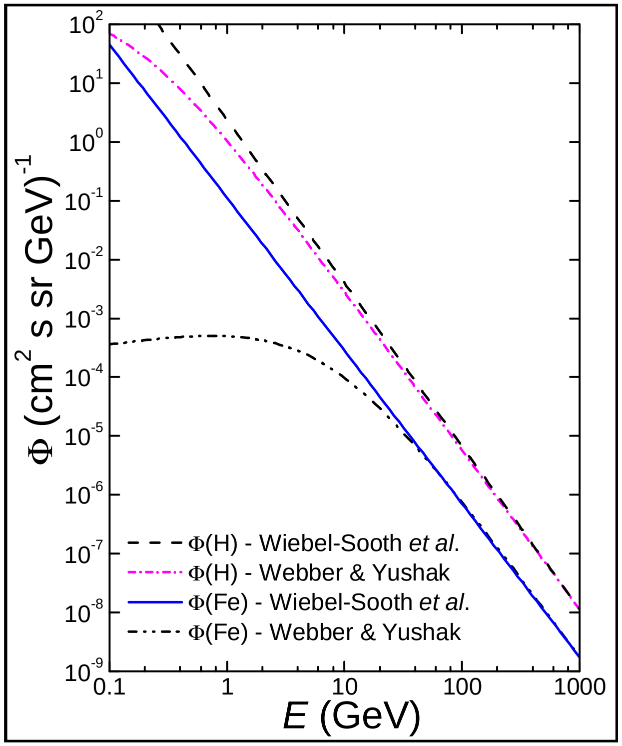
SiMAF

Amorphous Track Radius vs. Electronic Stopping Power



- 10 MeV results for forsterite fall on dE/dx curve
- R_{track} → amorphization dose
- Expect similar results at higher (CR) energies

New model of Cosmic Ray Flux



- Cannot compare to measurements including solar modulation … but …
- Modulation due to minimum escaping energy ~100 MeV

E.M. Bringa *et al.*, Astrophys. J. (2007)

+

=

Dose to amorphize forsterite "low" (~dose to amorphize SiO_2)

+

"Low dose" can be achieved in space

→

grain in space could be amorphized by CR

→

Astrophysical puzzle solved!

Example VI: Sputtering yield of porous solids
(Rodriguez-Nieva *et al*., *Astrophysical J. Letters*, 2011)

There are no reliable analitic or semi-analitic models of sputtering as a function of density for porous materials. “Exception”: Johnson, Icarus **78**, 206 (1989).

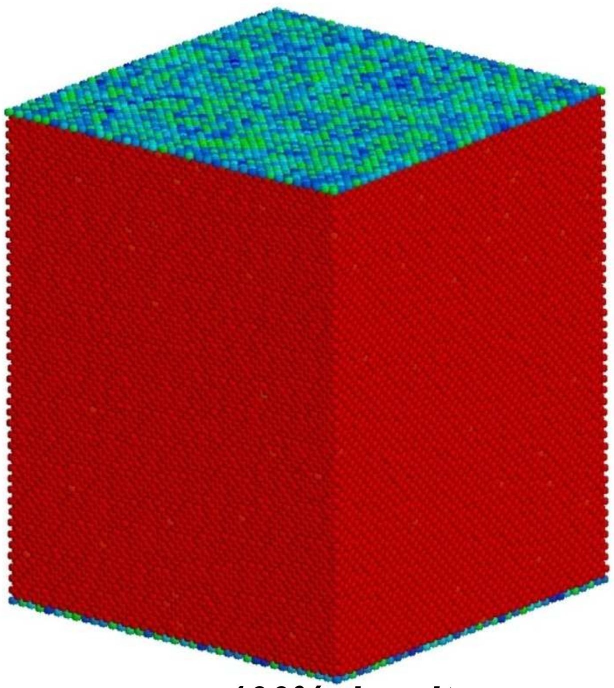
What can we expect? (Assume dE/dx does not depend strongly on geometry)

1) Fewer electronic excitations ➔ lower energy density ➔ lower yield

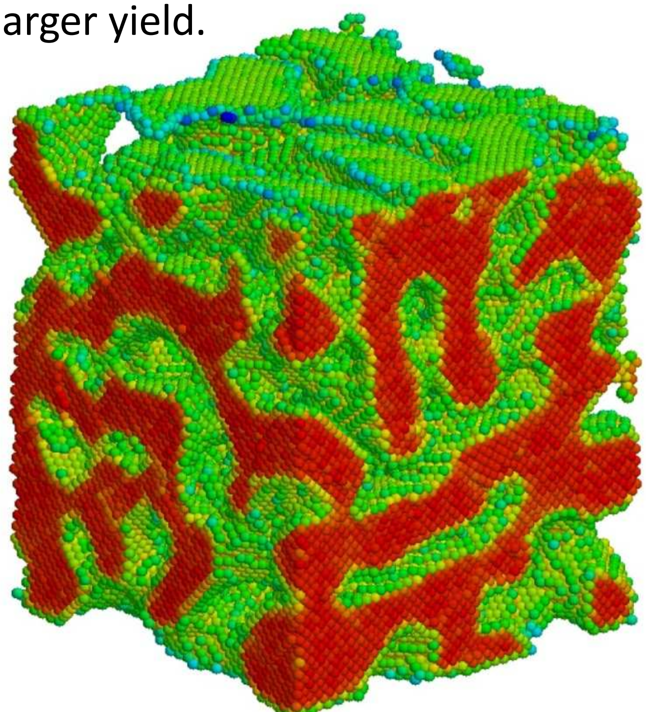
2) Larger effective surface ➔ higher yield

3) Atoms can be ejected from depth thanks to pores ➔

if sticking is large ➔ lower yield; if sticking is low ➔ larger yield.

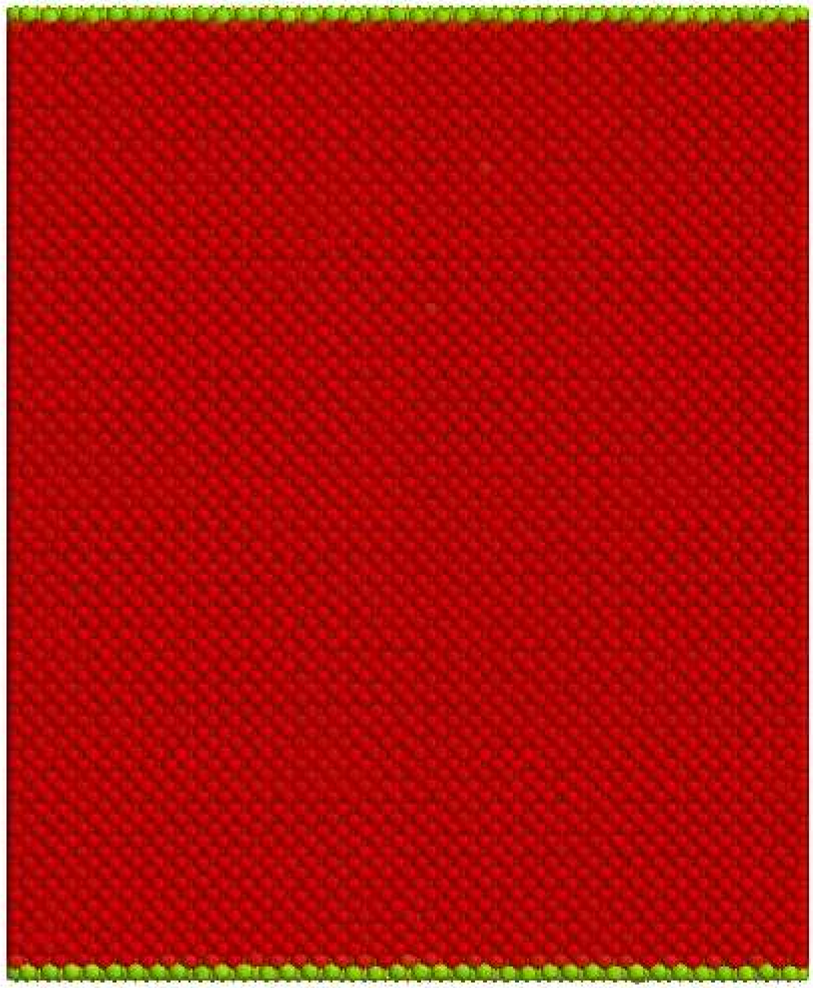


100% density

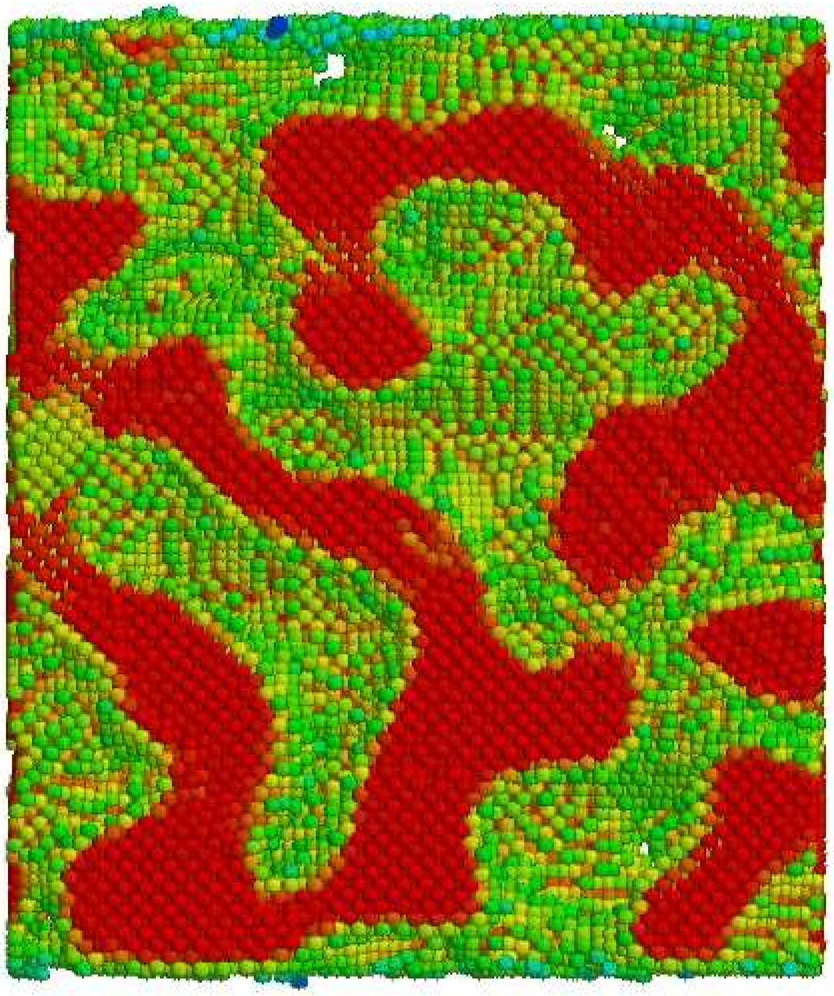


55% density

Sputtering from a "dense" solid



Sputtering yield from nanofoam ~sputtering for bulk solid



CONCLUSIONS

- **Simple models can account for many experimental results!**
- But **cannot** account for many other experimental results ….
- Poor understanding of: synergy between nuclear and electronic dE/dx + nuclear reactions, dE/dx at surfaces or nanostructures (islands, foams, nanoprecipitates, interfaces, etc.), charge-state effects (in dE/dx, ion ejection, charge exchange for both target & projectile, etc.), dE/dx for cluster projectiles, statistics of dE/dx and track size, etc.
- Beware of limitations due to system size and total simulated time!
- Empirical potentials offer severe constrains and have to be used with care:

  - where they were not intended to be used (phase transitions; high P/T; core-shell potentials for oxides problematic in radiation simulations).

  - where classical MD does not work properly (high P/T).

FUTURE- I

- Multi-scale models needed for improved simulations:

-coupling to FEM for larger system size;

-more general accelerated dynamics or KMC for defect evolution;

-coupling to MC/DFT/TB/TDDFT/naTB for better excitation treatment

-empirical potentials which depend dynamically on electronic state (high P/T, excitations, electron density – Khakshouri *et al*., PRB 2008-), etc.

- Better ion-electron models are already available and are discussed by several presentations in this workshop (Artacho, Caro, Correa, Fisher, Foulkes, Lu). The electron Force Field potential (eFF, Su & Goddard, PRL 2007) is another option for light elements.
- Still lacking reliable and efficient models for **swift heavy ions**.

FUTURE- II

- More CPU/**GPU** processing for MD parameter sweeping will speed up research, allowing for improved models, better potentials, and increasing statistics and parameter sweeping. LAMMPS/DL_POLY, etc. already have GPU versions.
- Need more links to experiments: measurement of surface and bulk defects (AFM/STM/TEM simulation –Victoria's talk-), IR spectra (Caturla *et al*.), X-ray diffraction simulation, mechanical properties, etc.
- Similarities with electronic excitations by photons (UV, lasers) should be exploited.
- **Need more experiments!**