Radiation Damage in Materials

3. Electronic stopping, SRIM, and swift heavy ion effects on materials
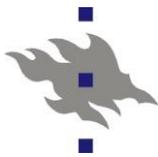
3.1. Electronic stopping power

■ Recall from previous section the definition of stopping power

$$S = -\frac{dE}{dx} = S_n + S_e + S_{reactions}$$

Log Stopping power

~ 1 keV/amu

~ 100 keV/amu

S_e

S_n

Bragg peak (not to be confused with x-ray Bragg peaks!

$S_{reactions}$

Log Energy
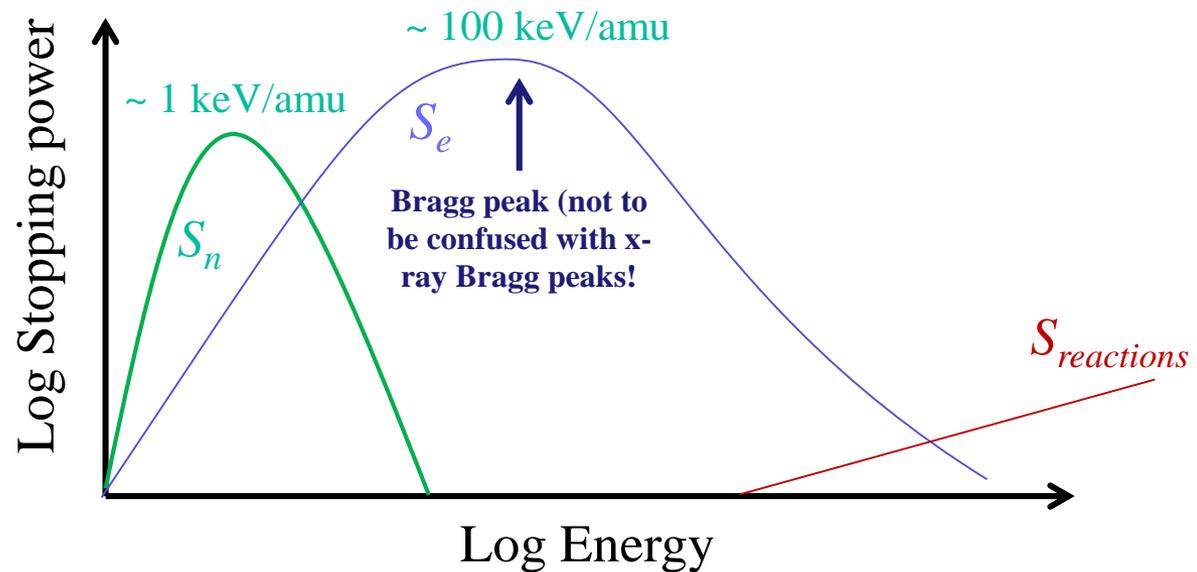
■ Now we will consider the electronic stopping power in more detail, especially its physical origins

Regimes of electronic stopping power

■ A more accurate description of the electronic stopping over energy regimes.

■ These are marked as A, B, C and D in the figure

■ These are described next **in order of good understanding:**

D->B->C->A
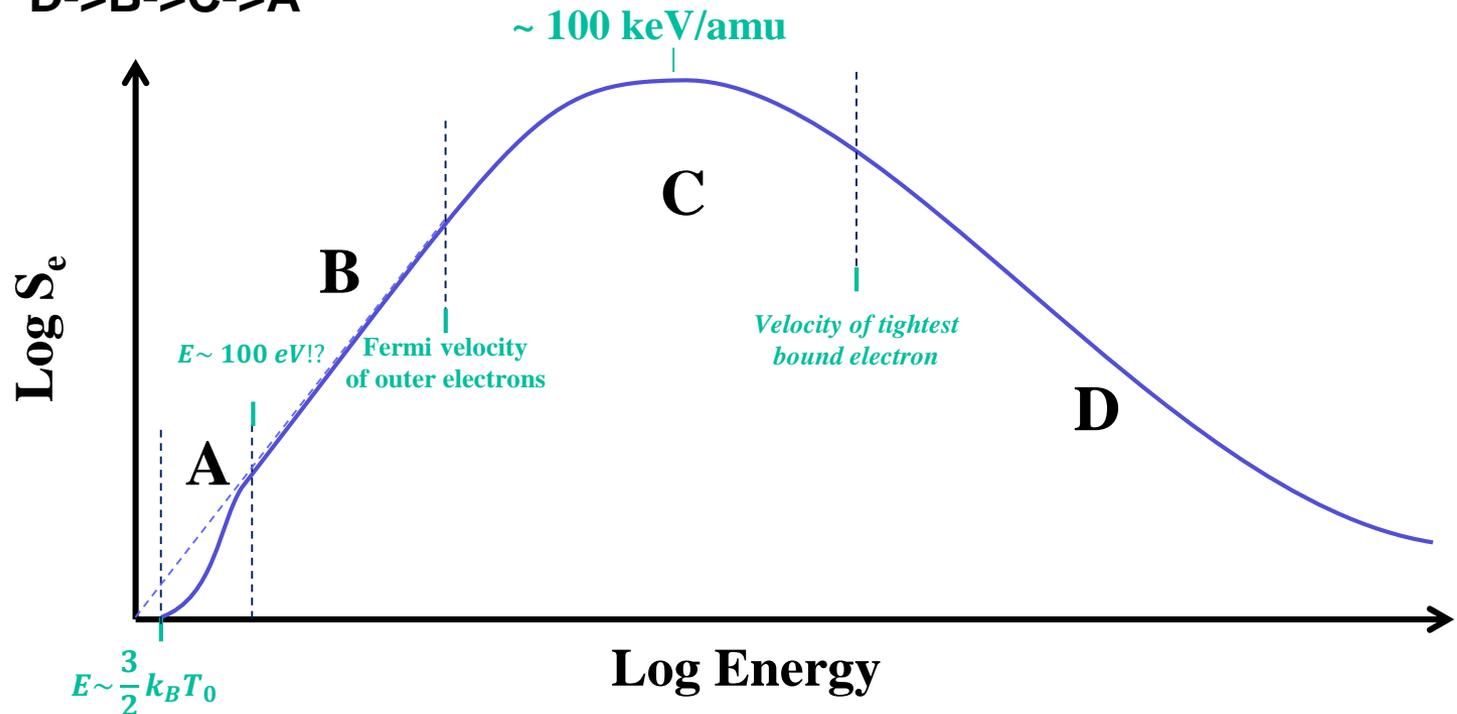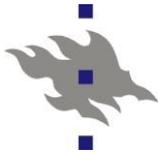
Regime D: Bethe-Bloch

- The highest-energy regime can be well understood based on the Bethe-Bloch theory, derived already in the 1930's

Plot with axes "Log S_e" (vertical) and "Log Energy" (horizontal). Curve rises through regions A, B, peaks at C (~ 100 keV/amu), and falls through D. Annotations: $E \sim \sim \frac{3}{2} k_B T_0$, $E \sim 100\ eV!?$, Fermi velocity of outer electrons.

- At these high energies, the moving ion is fully or highly charged and does not change charge state

- The Bethe-Bloch equations derive the stopping power quantum mechanically for a charged particle moving in a homogeneous electron gas

  - I.e. consisting of all electrons of the material as if they were evenly distributed

  - Atomic structure of the sample ignored in these equations!

    - This is not accurate, but for high enough energy works as a good 1st approximation
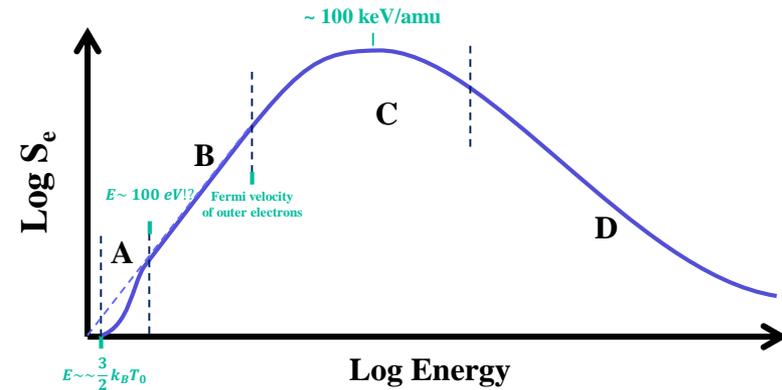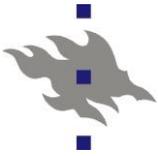
Regime D: Bethe-Bloch equations

- The basic equation is relatively simple [Was]

$$\left(-\frac{dE}{dx} \right)_e = \frac{N2\pi Z_1^2 Z_2 \varepsilon^4}{E_i} \frac{M}{m_e} \ln\left(\frac{\gamma_e E_i}{\bar{I}} \right) = \frac{2\pi N Z_1^2 M \varepsilon^4}{m_e E_i} B$$

where

$$B = Z_2 \ln\left(\frac{\gamma_e E_i}{\bar{I}} \right)$$

is known as the stopping number, Z_1 is the atomic number of the ion, Z_2 of the material, N is the atomic density of the material, ε is the electron charge e, I is the mean excitation energy level which to a first approximation is 11.5 eV Z_2, and

$$\gamma_e = \frac{4m_e M}{(m_e + M)^2}$$

- For relativistic velocities

$$B = Z_2 \left\{ \ln\left(\frac{\gamma_e E_i}{\bar{I}} \right) - \ln\left(1 - \beta^2 \right) - \beta^2 \right\}$$
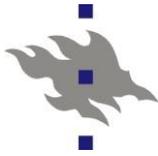
Regime B: velocity-proportional regime

- In regime B the stopping is almost exactly linearly proportional to ion velocity,

$$S_e \propto v$$

- This regime has an upper limit at the Fermi velocity of the slowest (outermost) electron of the material

- The direct proportionality to velocity agrees well with experiments, and has been derived in several different ways

  - By Fermi and Teller using Fermi velocity [Phys. Rev. 72 (1947) 399]
  - By the Lindhard-Sharff-Schiott (LSS) theory [Mat. Fys. Medd. Dan. Vid. Selsk. 33 (1963)
    This reference gives analytical equations for the stopping power in this "Lindhard regime"
  - Quantum mechanically by Echenique-Nieminen-Ritchie [Solid State Comm. 37 (1981) 779].

- Also the most modern electronic-structure calculations give about the same result (some give $S_e \propto v^{0.9}$)
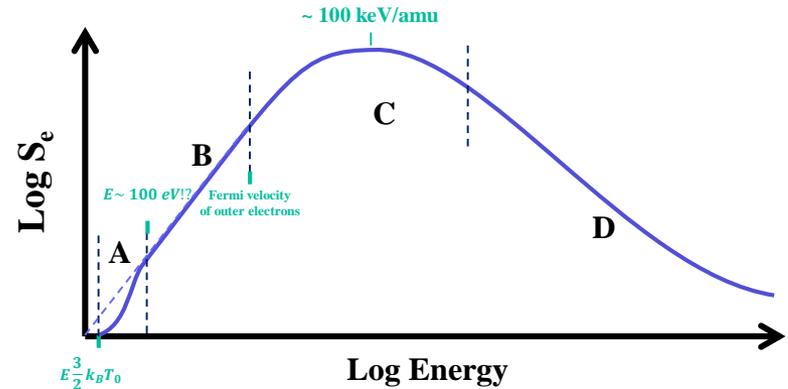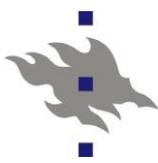
Regime B:
Fermis explanation to low-E stopping power

- The paper by Fermi and Teller provides an intuitively clear explanation for why low-E electronic stopping is directly proportional to the ion velocity v:
- The following texts are direct quotes from the paper:
  - "Consider an ion with velocity v moving in a degenerate (0 K) Fermi gas. **If any single electron transfers momentum to it in a collision** (slowing the ion down), its own momentum/velocity of course also should change. "

Metal with free electrons

Ion and its electrons
moving with velocity v

V →
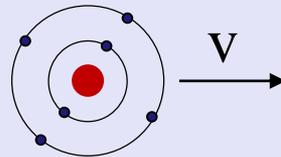
Since v is very high,
electrons in solid
are effectively at rest
and in equilibrium
when the ion and its electrons
collide with them

[E. Fermi and E. Teller, The capture of negative mesotrons in matter, Phys. Rev. 72 (1947) 399]

Regime B:
Fermis explanation to low-E stopping power

■ The crucial idea is: "Only electrons with a velocity within v of the Fermi velocity v_F in one dimension (the moving direction of the ion) can contribute to the stopping. This is because electrons below v_F-v in velocity could only gain [at most] v in velocity and hence be excited to an already filled state. The latter is of course forbidden by the Pauli principle. "

State occupation $n(v)$

Electrons that cannot be excited

Electrons that can be excited

v v_F-v v_F
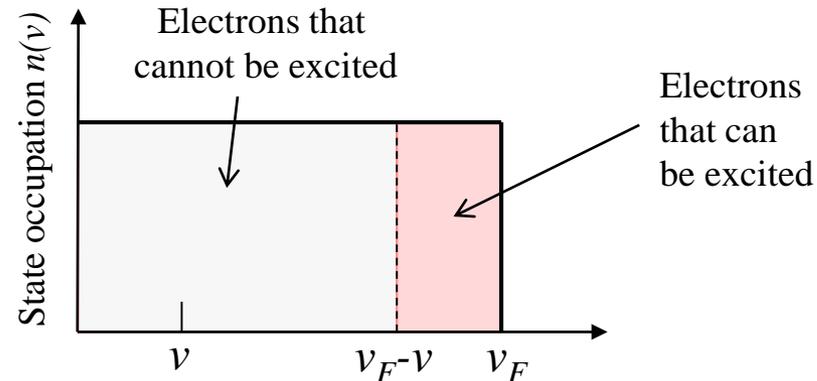
■ "Electrons within v of v_F, on the other hand, can be excited above the Fermi level to unoccupied states. Hence the higher v is, the more electrons can contribute to the stopping. "

   ■ "More specifically, the amount of electrons in a unit volume with velocity within v of v_F is proportional to v simply because the density of states in 1D is $2\pi/L$ so an integral from v_F to v_F - v is proportional to v. "

[E. Fermi and E. Teller, The capture of negative mesotrons in matter, Phys. Rev. 72 (1947) 399]
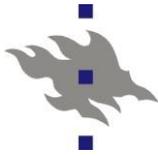
Regime C: the complex one…

■ The maximum region in the stopping power is a regime where the moving ion is partly ionized, and its charge state fluctuates

■ I.e. it undergoes stochastic charge exchange processes with the atoms of the material

■ There is no simple analytical equation that can describe this region fully reliably

[If interested in the existing models, see chapter 4 in the "SRIM book" described in section 3.3.
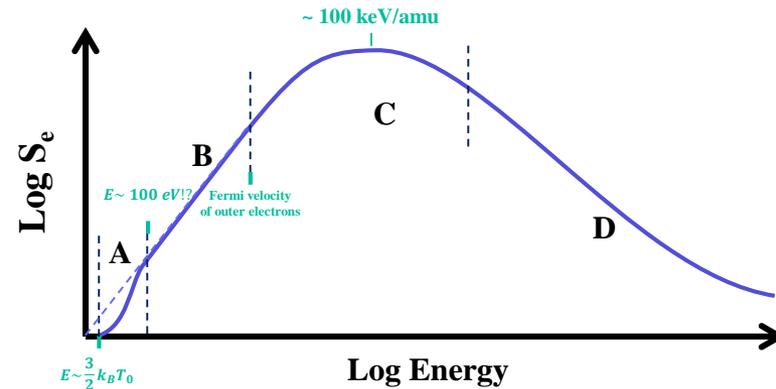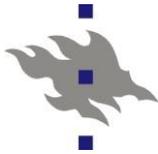
Regime C: empirical

■ The best way to treat the stopping in regime C is to try to find experimental data for it, and if available, use that directly

■ This energy regime is one of the easiest to measure experimentally and hence plenty of data does exist

http://www.srim.org/SRIM/SRIMPICS/STOP-TGTS/STOPxx74.gif
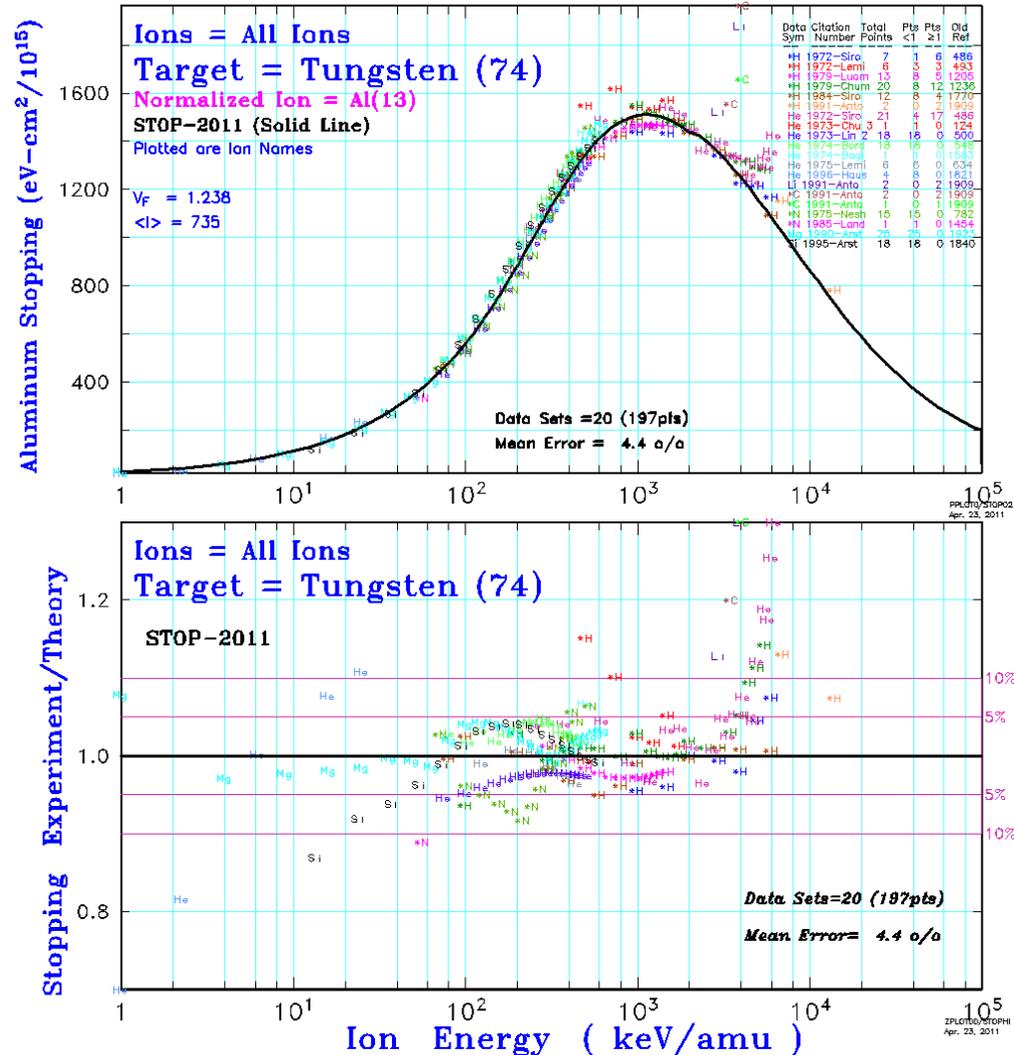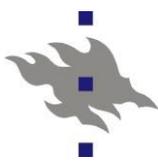
Regime C: modelling

- The SRIM semi-empirical model does give data for this regime, but it is not so reliably (~20% deviations common)
- There are modern simulation codes that can handle the regime C stopping fairly well theoretically
- The best developed is probably CaSP by Gregor Schiwietz and P. L. Grande, http://www.casp-program.org/, reference e.g. [Phys.Rev. **A58**, 3796 (1998)]
- Sample CaSP results compared to experiment:

[Gregor Schiwietz and P. L. Grande, PHYSICAL REVIEW A **84**, 052703 (2011)]
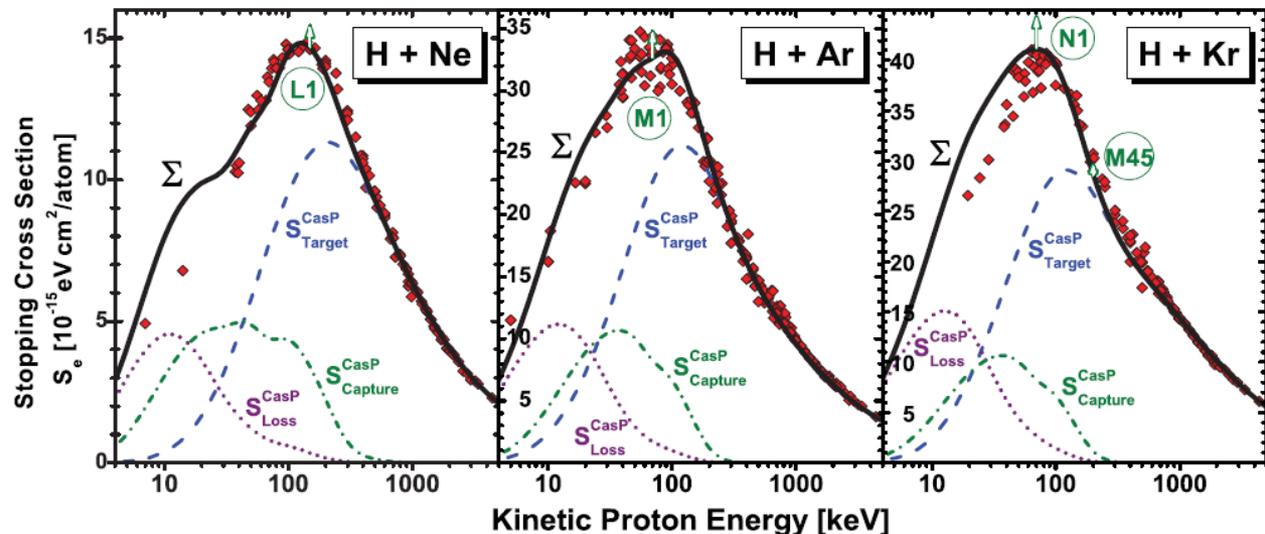
Regime A: the least well known

- The lowest-energy regime is actually the least well known

- The simple theories predict that $S_e \propto v$ for all energies, but this is absurd when the atom velocity becomes thermal: atoms in equilibrium do not experience any electronic stopping

  - If $S_e \propto v$ would be true also near equilibrium, all atom systems would be quenched down to 0 K in nanoseconds, which is obviously not true.

Figure labels: Log S_e, Log Energy, B, A, $E \sim 100\ eV!?$, Fermi velocity of outer electrons, $E \sim \frac{3}{2} k_B T_0$
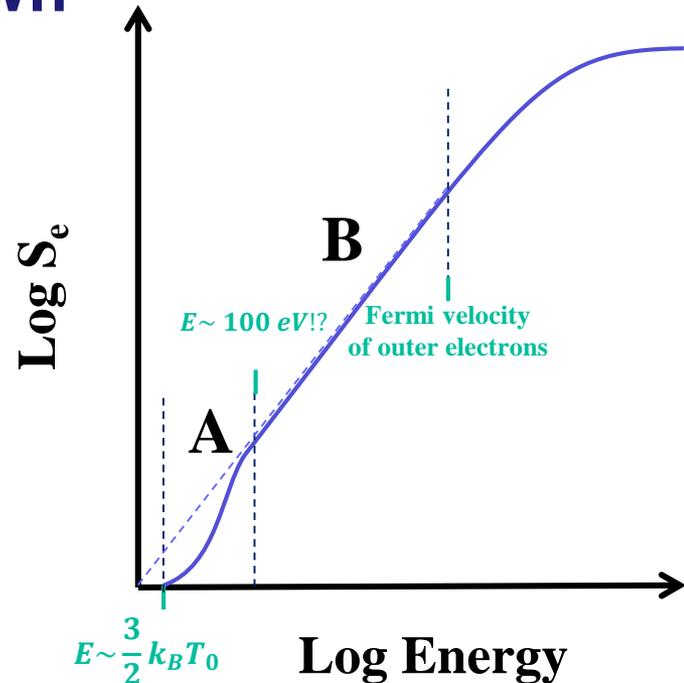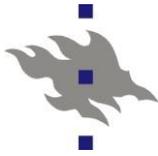
Regime A: experimental and simulation data

- Experiments show that indeed the electronic stopping becomes weaker than the direct proportionality to velocity at low velocities

- Plotted in the adjacent figures is Q, which is defined by $S = Q v$ => constant Q means velocity proportionality.

- Advanced quantum mechanical (so called time dependent density functional theory) calculations can reproduce this
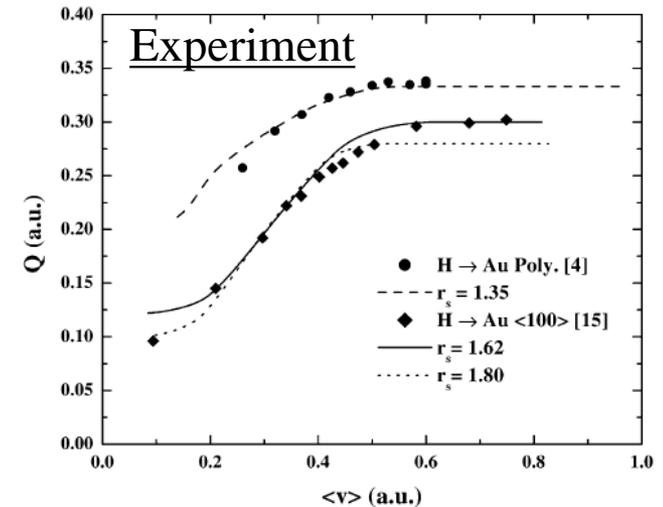
[Valdes et al, Nuclear Instruments and Methods B 193 (2002) 43]
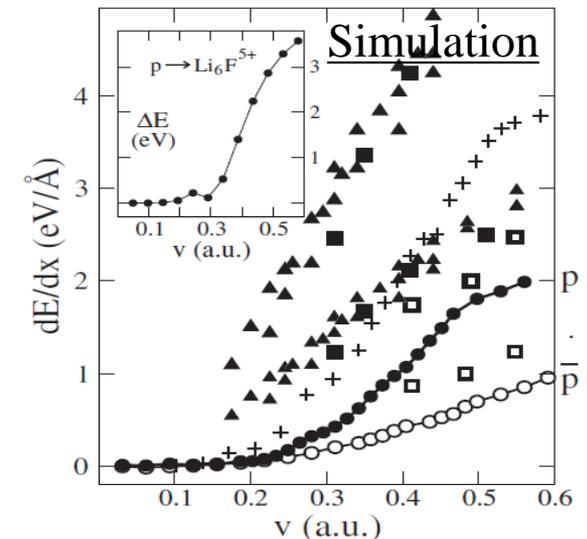
[Pruneda et al, PRL **99,** 235501 (2007)]
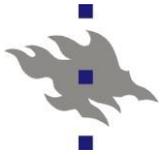
Regime A: uncertainty remains…

- Not all metals show this behaviour, however.

- The reason to the lowering can be qualitatively understood based on the electron density of states near the Fermi level:
    - In insulators there are no electrons, and the stopping will indeed have a threshold
    - Metals have electrons, but if the density of states is low near the Fermi energy, the stopping will be reduced compared to that at higher velocities

- However, there are extremely few experiments in this regime, and none for projectiles heavier than He. Hence for heavy ions/recoils it is not really known what the low-energy limit is
    - Also very difficult to model theoretically

Regime A and the electron-phonon coupling

- In general, in non-equilibrium thermodynamic systems, the ions (atom cores) and electrons can sometimes be decoupled from each other such that they have different temperatures, T_i and T_e
    - This can be achieved with some external disturbance, e.g. laser or ion irradiation
- **Electron-phonon coupling** (*elektron-fonon-koppling, elektroni-fononi-kytkentä*) means quite generally in physics how strongly the ionic and electronic subsystems are coupled to each other by a coupling constant G
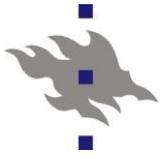
Electron-phonon coupling equation

- This can be mathematically described with two coupled differential equations:

$$C_e(T_e)\frac{\partial T_e}{\partial t} = \nabla[K_e(T_e, T_l)\nabla T_e] + \text{G}(T_e)(T_e - T_l) + S_e(\vec{r}, t)$$

$$C_l(T_l)\frac{\partial T_l}{\partial t} = \nabla[K_l(T_l)\nabla T_l] + \text{G}(T_l)(T_e - T_l) + S_l(\vec{r}, t)$$

Here C and K are the thermal capacity and conductivities of each subsystem e and l separately, T_e and T_l are the temperatures and G is the electron-phonon coupling (which may depend on the local temperature)

- S are source terms of the disturbance putting the two subsystems out of balance: S_e is the source from electronic stopping, S_l is the source in case the lattice is heated before electron-phonon coupling e.g. from ballistic collisions

[Lin and Zhigilei, Phys. Rev. B **77**, 075133 2008]
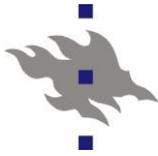
Regime A: the lowest energy limit

■ Some serious thought of the physics involved in stopping makes it clear that the whole concept of electronic stopping makes sense only when the ion/atom moves more rapidly than the thermal velocities

■ When the electronic and atomic subsystems start to behave like a thermodynamic system, electron-phonon coupling starts to occur (the electronic stopping acts as the source term S

  ■ When finally $T_e = T_l$, **there is no longer any electronic stopping**
  ■ This is indicated as the lower-limit of $E \sim \frac{3}{2} k_B T_0$ in the graph

■ There is some very recent work to link the two regimes:
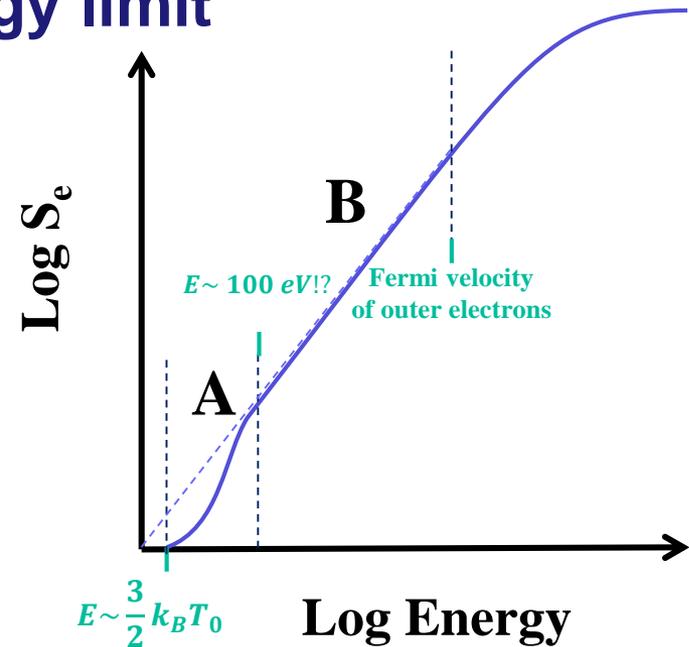
[A. Tamm et al, Phys. Rev. Lett. 120, 185501 (2018)]
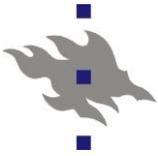
3.2. How to use electronic stopping power?

- If the stopping power would be constant $= S_0$, its use would be very simple:

$$\frac{\Delta E}{\Delta x} = -S_0 \Rightarrow \Delta E = -S_0 \Delta x$$

  i.e. for a path length Δx travelled in a material, the ion loses ΔE of energy.

- Now that in reality S is not really constant in any wider energy range but is $S = S(E)$, one needs to integrate to get the energy loss over a finite energy range:

$$\frac{dE}{dx} = -S(E) \Rightarrow \Delta E = \int_0^x -S(E)dx$$
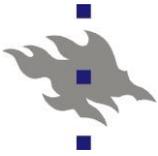
Range calculation

■ The ion penetration depth (mean range) can, if an ion with initial energy E_0 would travel fully straight, calculated directly from the stopping using

$$\frac{dE}{dx} = -S(E) \Rightarrow dx = -\frac{dE}{S(E)} \Rightarrow R = \int_0^R dx = \int_0^{E_0} \frac{dE}{S(E)}$$

■ **As an example**, for protons electronic stopping dominates over nuclear for all energies, and one could use the linear velocity dependence model $S(E) = k\, E^{1/2}$. In this case the integral can be done analytically and one obtains

$$R = \int_0^R dx = \int_0^{E_0} \frac{dE}{kE^{1/2}} = \frac{2}{k}\sqrt{E_0}$$

Range concepts

■ However, this calculation **has a major weakness**: the stopping power is always along the ion, **path length** R and the ion due to nuclear collisions almost certainly does not move in a straight path

■ In fact one can distinguish between different range concepts:

■ R_Z = depth coordinate of final ion position

■ R_p = projected range

(for perpendicular impacts

= penetration depth R_Z)

■ R_c = chord range

■ R = total path length

■ $R_\perp$ = range perpendicular

to initial direction (lateral range)

[Picture from Was book]

[These concepts date back to Lindhard, Scharff, Schiott 1963]
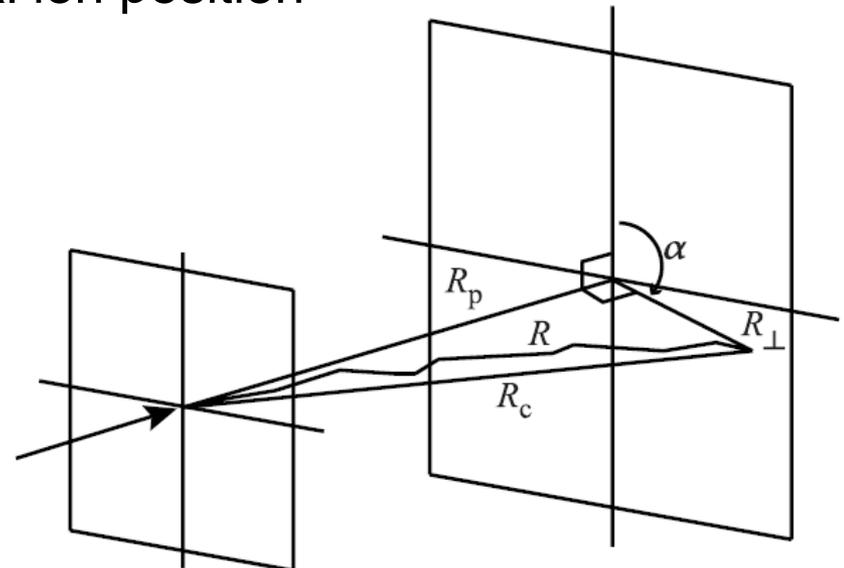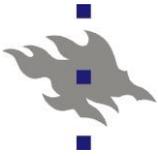
Illustration of difference of range concepts

- The following figure gives actual ion trajectories for 10 keV Si ions impacting on Si at 20 degrees off-normal

  - 100 distinct trajectories
  - Projection of 3D ion paths to xy plane
  - Colors give kinetic energy of ions

- Note how the path ranges are much longer than any of the others

100 trajectories of 10 keV Si ions impacting on Si at theta=20
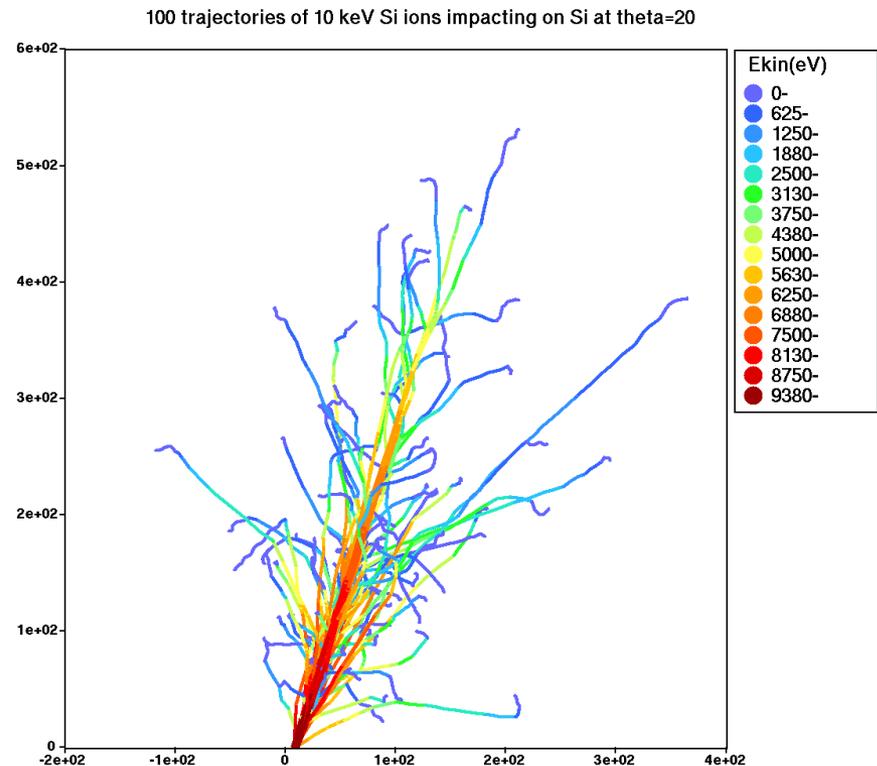
[These was obtained with a molecular dynamics range calculation (MDRANGE) that can simulates the ion movement stepwise and hence can also sum up the path range. Kai Nordlund 12.4.2020]
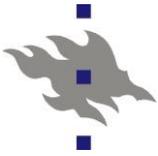
Range calculation: distributions

■ Due to this, the simple equation

$$\frac{dE}{dx} = -S(E) \Rightarrow dx = -\frac{dE}{S(E)} \Rightarrow R = \int_0^R dx = \int_0^{E_0} \frac{dE}{S(E)}$$

is useful **only as an estimation of the maximum range**, i.e. the range of those ions that happen to travel in a completely straight path

■ In most cases, due to scattering, the mean range is much less than the maximum range
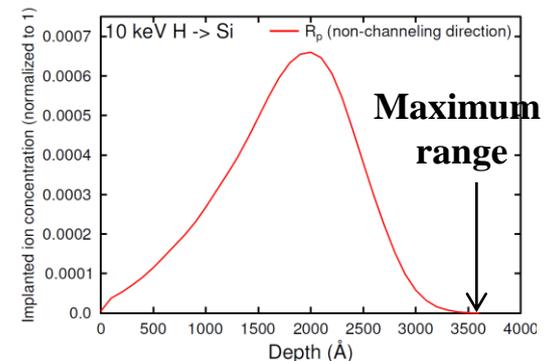
Schematic from section 1

Example for 10 keV H in Si

[Data from MDRANGE with zbl96 electronic stopping power. Kai Nordlund 12.4.2020]

Range calculation: distributions

- For the case of 10 keV Si ions in Si (20 degrees off-normal) the range profiles defined with the different range concepts differ in a natural way:

[Data from MDRANGE with zbl96 electronic stopping power. Kai Nordlund 12.4.2020]
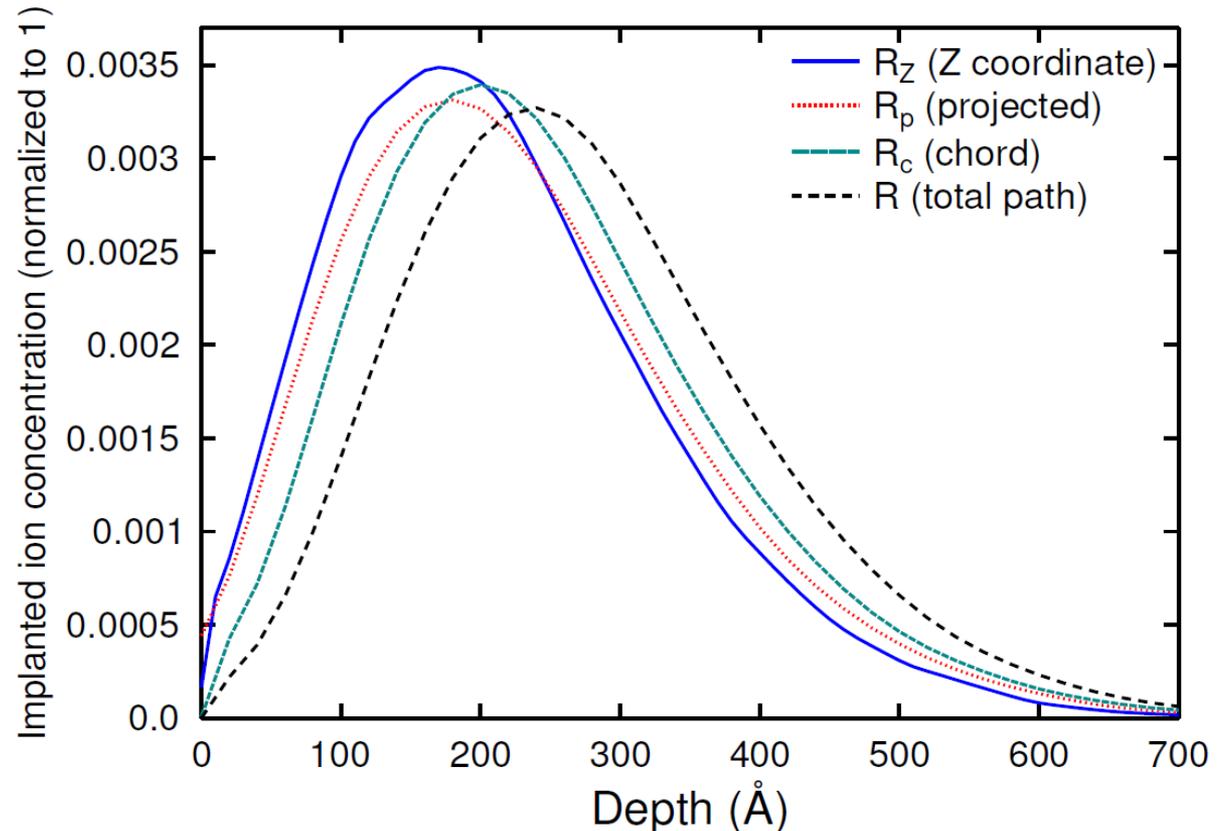
Range concepts translated to Finnish/Swedish

- R_p = projected range (*projicerad räckvidd / projisoitu kantama*)

- R_c = chord range (*strängräckvidd / jännekantama*)

- R = total path length (*total väglängd / kuljettu kokonaismatka*)

- $R_\perp$ = range perpendicular to initial direction (lateral range) (*räckvidd vinkelrät mot inkommande riktningen, lateral räckvidd / kantama kohtisuoraan sisääntulosuuntaa vastaan / lateraalinen kantama*)

Analytical range calculations

- Out of these, the standard one in use is the (mean) projected range $\overline{R_p}$

- But for non-perpendicular irradiation also the mean penetration depth $\bar{Z}$ is for practical reasons often used

$$\bar{Z} = \overline{R_p} \cos(\theta)$$

  - Difference a factor of cos(θ)

- Lindhard-Sharff-Schiott (LSS) theory [Mat. Fys. Medd. Dan. Vid. Selsk. 33 (1963) 1] developed ways to estimate the $\overline{R_p}$ from the stopping

  - But nowadays most people use BCA simulations to calculate range distributions, so these are no particularly important anymore
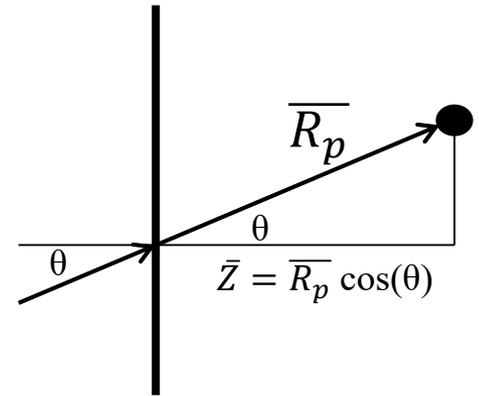
Local vs. nonlocal stopping models

■ The models as described above were presented as if the electron density would be constant everywhere in a solid.

■ In reality this is of course not true: the density is orders of magnitude higher around the atom cores

■ Some models do take this into account: so called **local models** for electronic stopping describe it as a sequence of atomic collisions, where the stopping is atom-specific

FIG. 1. Electron distribution of silicon in a (110) plane. [Sillanpää, Nordlund, Keinonen, Phys. Rev. B **62**, 3109 (2000)]

   ■ For instance the Firsov model [Kishinevskii, Bull. Acad. Sci. USSR, Phys. Ser. 26 (1962) 1433]

■ Others, like LSS and SRIM, use a homogeneous density
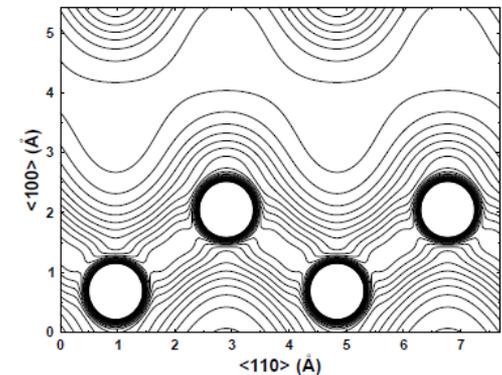
Local models and ion channeling

- For ions moving in a 'random' direction the nonlocal models generally work well

- However, an ion moving in a well-defined crystal direction with low electron density will obviously never experience the higher density around the atom cores, and using the average density can give badly wrong results

FIG. 1. Electron distribution of silicon in a (110) plane.

[Sillanpää, Nordlund, Keinonen, Phys. Rev. B **62**, 3109 (2000)]

  - This kind of an ion is called **channeled** (*kanaliserad / kanavoitunut*) as it moves in a crystal 'channel'

- For these cases using a local model is crucial
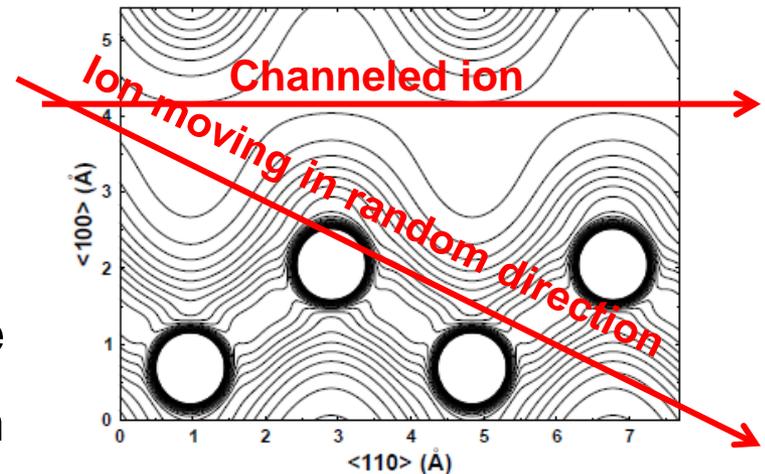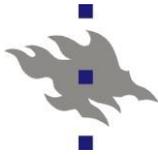
Results for a fully local model

- Local models can be atom-specific, or take into account the full 3D electronic structure of the material

- Implementing the latter kind of model based on the Echenique-Nieminen-Ritchie stopping theory, Sillanpää, et al. obtained very good agreement with ion ranges for both random and channeled directions in Si:
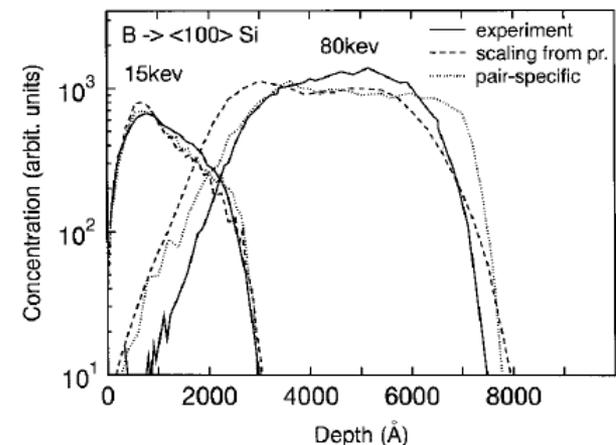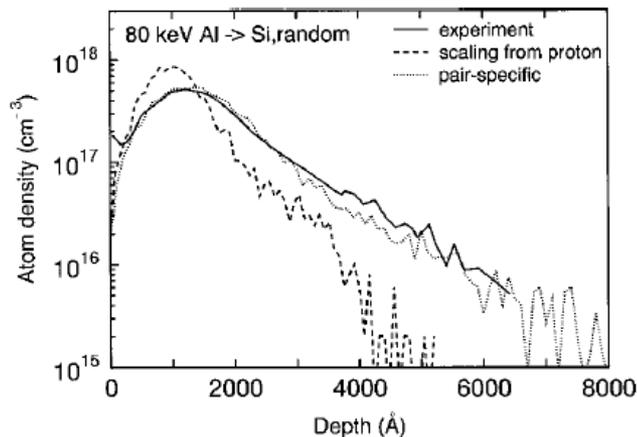
[Sillanpää, Peltola, Nordlund, Keinonen, Puska , papers e.g. Phys. Rev. B **62**, 3109 (2000) and Phys. Rev. B **63**, 134113 (2000)]
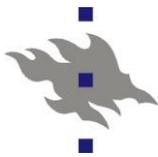
3.3. Ion channeling from nuclear collisions

- **The channeling is also a nuclear collision effect**
    - Ions in a channel are focused by the nuclear collisions
    - This has a well-established theory that describes the channeling via so called continuum potentials
        - Good review: Gemmell, Rev. Mod. Phys. 46 (1974) 129
- **Both the nuclear and electronic effects for channeling lead to enhancements of the ion range in channeled direction**
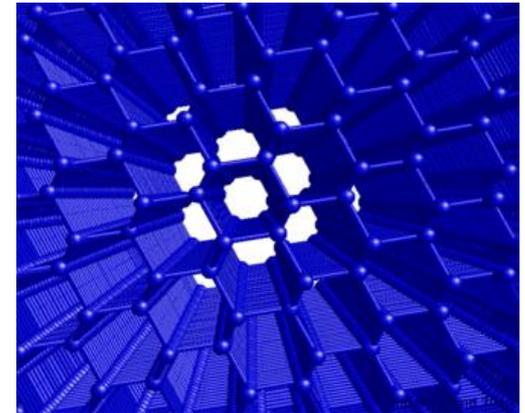
An about 12 nm thick silicon crystal viewed down the 110 crystal direction
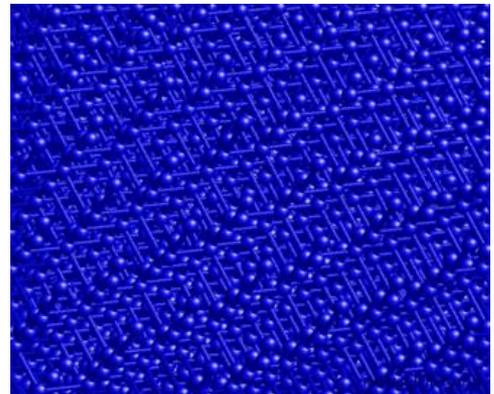
Same Si crystal as above viewed from a randomly rotated direction [Wikipedia by me]
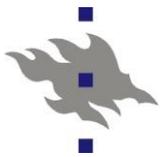
Channeling illustration

Ions in channeling direction

30 individual 1 keV Si in Si ion trajectories, theta=45, phi=0
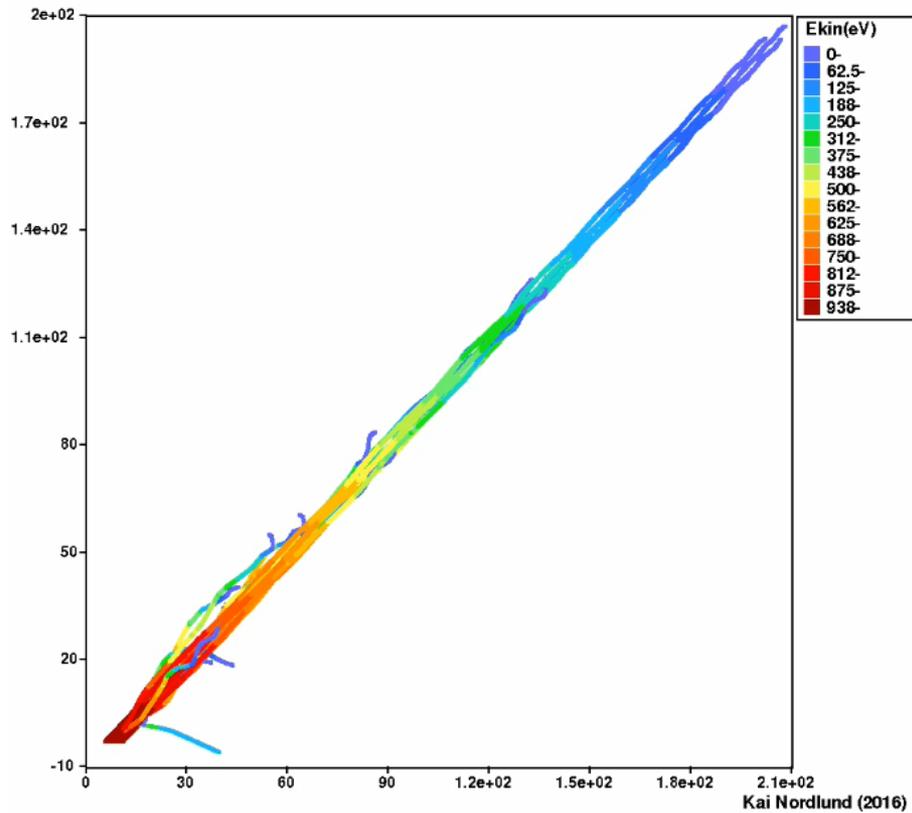
Ions in non-channeling direction

30 individual 1 keV Si in Si ion trajectories, theta=30, phi=0
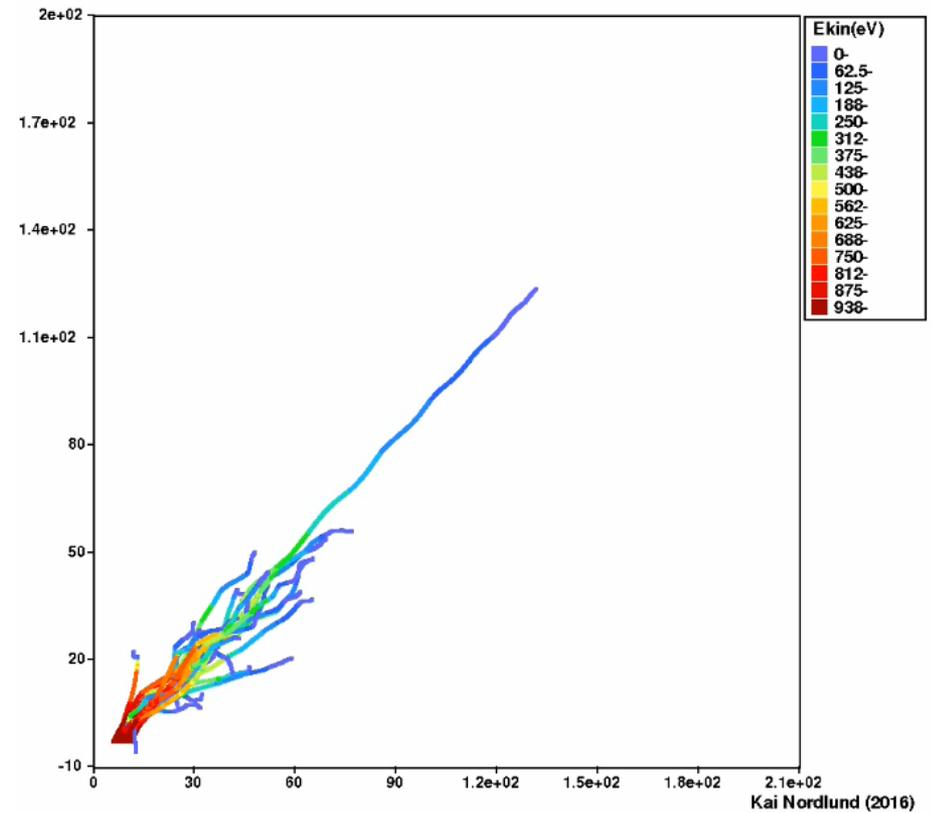
Channeling illustration (trajectory animation)

Ions in channeling direction

100 individual 1 keV Si in Si ion trajectories, theta=0, phi=0
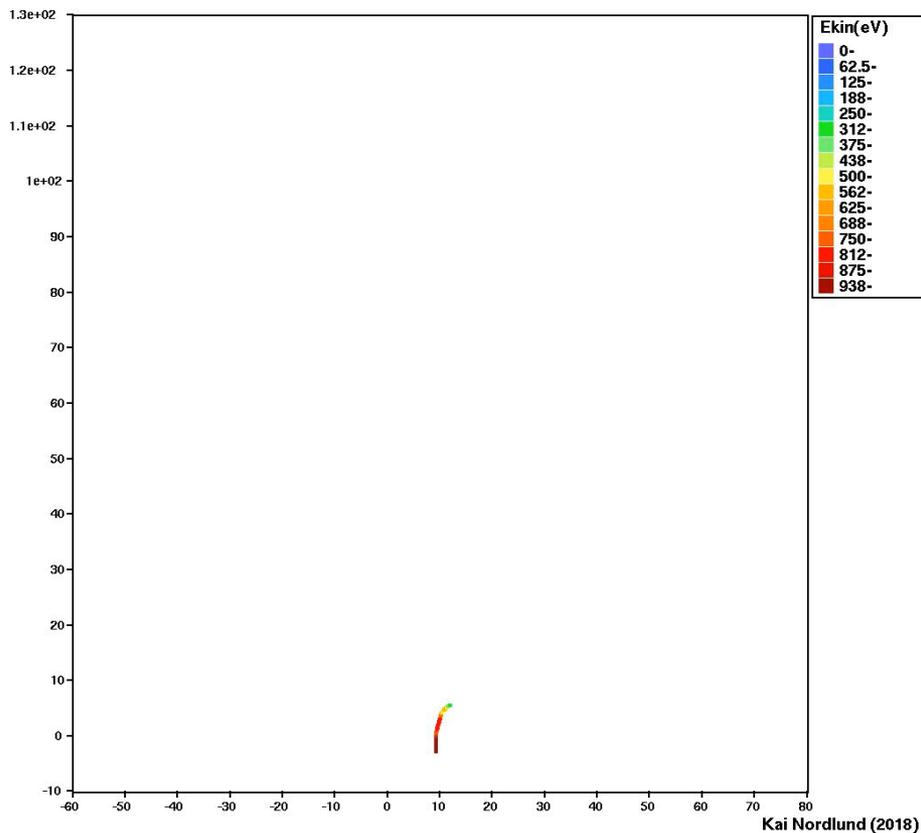
Ions in non-channeling direction

100 individual 1 keV Si in Si ion trajectories, theta=7, phi=27
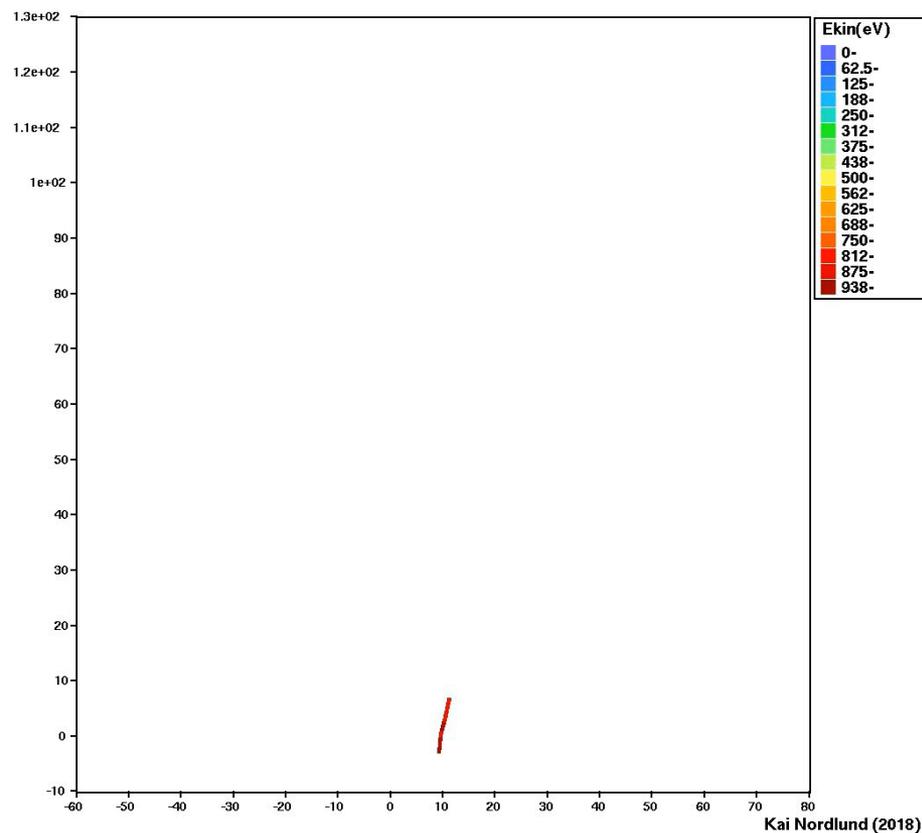
Ion channeling from nuclear collisions

- The magnitude over different crystal direction can be easily seen from so called "channeling maps"
  - These plot as a color scale the ion mean range as a function of the incoming ion beam direction (θ, φ) over all crystallographically nonequivalent directions

θ = polar angle
φ = azimuthal angle

Surface normal 001
010
100

1.7 MeV Au on 20 nm Au foil

E_dep(eV)
0-
18800-
37500-
56300-
75000-
93800-
1.12e+05-
1.31e+05-
1.5e+05-
1.69e+05-
1.88e+05-
2.06e+05-
2.25e+05-
2.44e+05-
2.62e+05-
2.81e+05-

Azimuthal angle

Polar angle

150 keV W on W

Rmean(Å)
0-
75-
150-
225-
300-
375-
450-
525-
600-
675-
750-
825-
900-
975-
1050-
1130-

Azimuthal angle

Polar angle
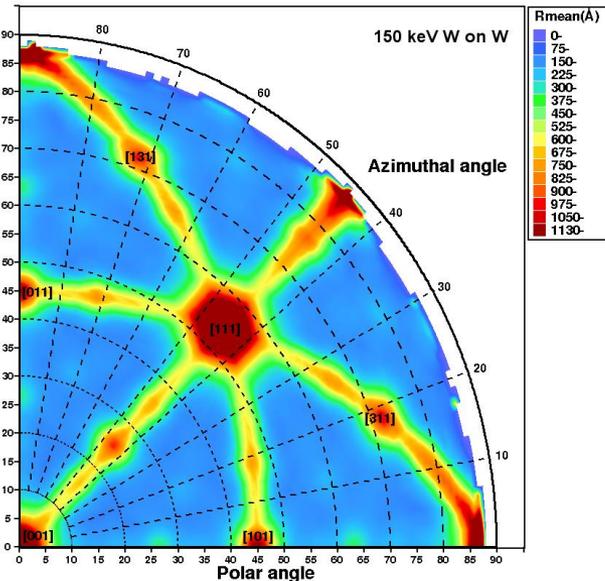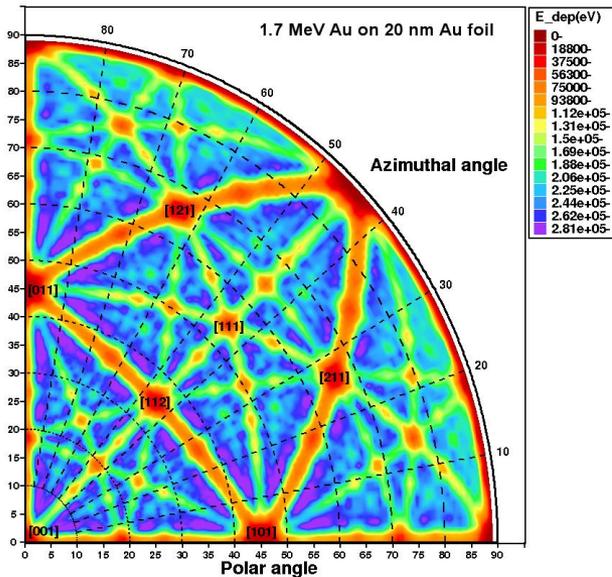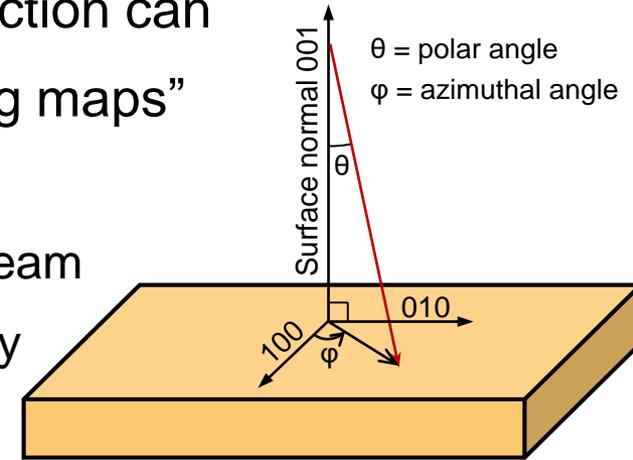
**RED regions:
Strong channeling
PURPLE regions:
No channeling or
blocking**

[More maps: K. Nordlund, F. Djurabekova, and G. Hobler. Phys. Rev. B, 94:214109, 2016]
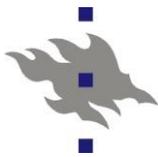
Analysis of fraction of channeling directions

- From the channeling maps simulations or channeling theory, the fraction of channeling directions can be systematically analyzed

  - Result: huge fraction of all incoming ion directions are channeling. This implies that in polycrystalline materials, ranges are enhanced

[K. Nordlund, F. Djurabekova, and G. Hobler. Phys. Rev. B, 94:214109, 2016]
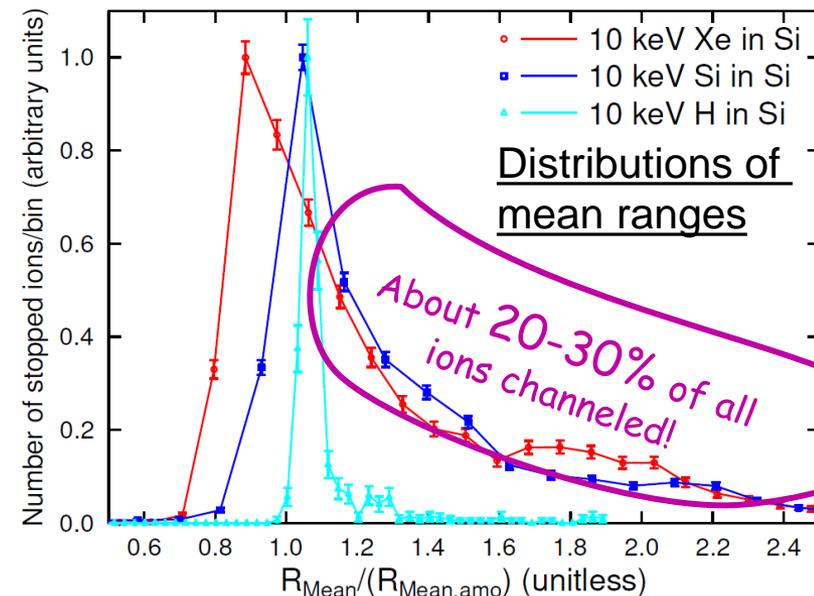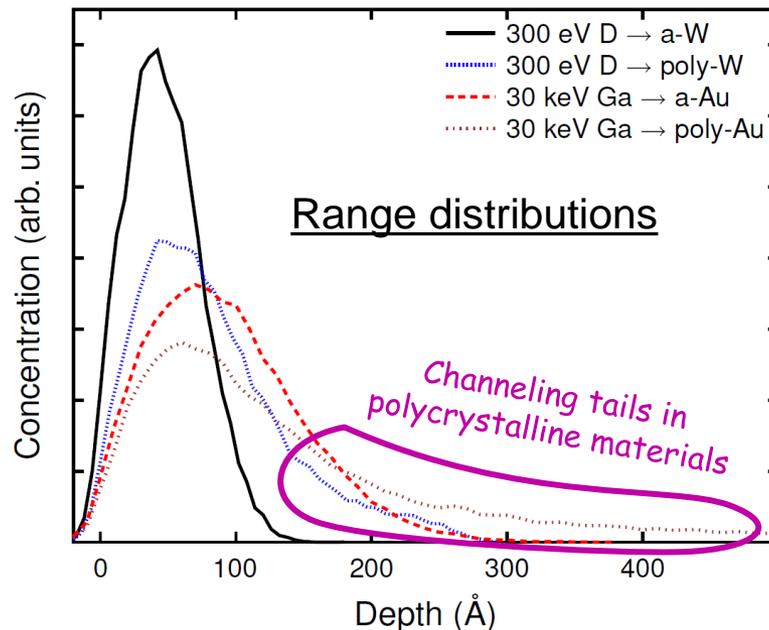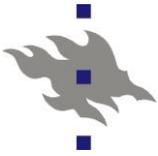
3.4. SRIM and electronic stopping databases

- There are two major sources of electronic stopping:

  - The one by the SRIM organization, www.srim.org.
    - **SRIM stands for "The Stopping and Range of Ions in Matter"** and is also the name of an ion stopping software
    - SRIM is (as of this writing in 2020) still run by Jim Ziegler, who worked earlier at IBM research and spent much of his career developing electronic and nuclear stopping models
    - A major collection of stopping data is freely available at the SRIM web pages

  - Documentation: several publications, material on the web site, and the two books:
    - "The ZBL book"; J. F. Ziegler, J. P. Biersack, and U. Littmark. The Stopping and Range of Ions in Matter. Pergamon, New York, 1985.
    - "The SRIM book", SRIM – The Stopping and Range of Ions in Matter, J. F. Ziegler, J. P. Biersack and M. D. Ziegler, SRIM Co, www.SRIM.org

  - **The International Atomic Energy Agency IAEA** maintains another database: https://www-nds.iaea.org/stopping/
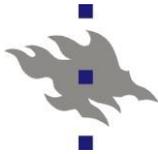
Examples of data from SRIM

- Normalized data for stopping of all ions in Carbon
- Each atom name is a data point is a measurement!
- Lower part shows deviation from SRIM semi-empirical model
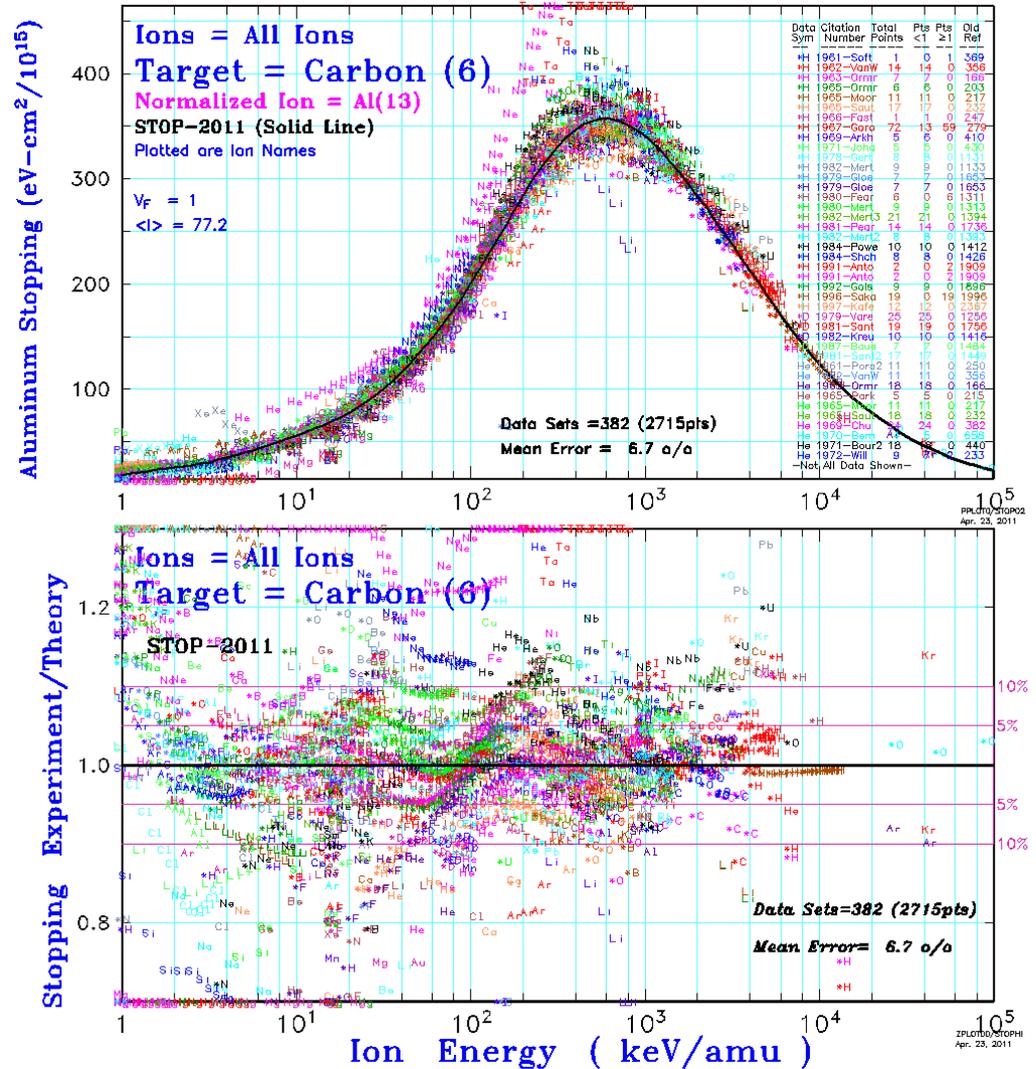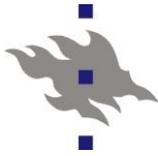
Examples of data from SRIM

■ Same for

Copper

[http://www.srim.org/SRIM/SRIMPICS/STOP-TGTS/STOPxx29.gif]
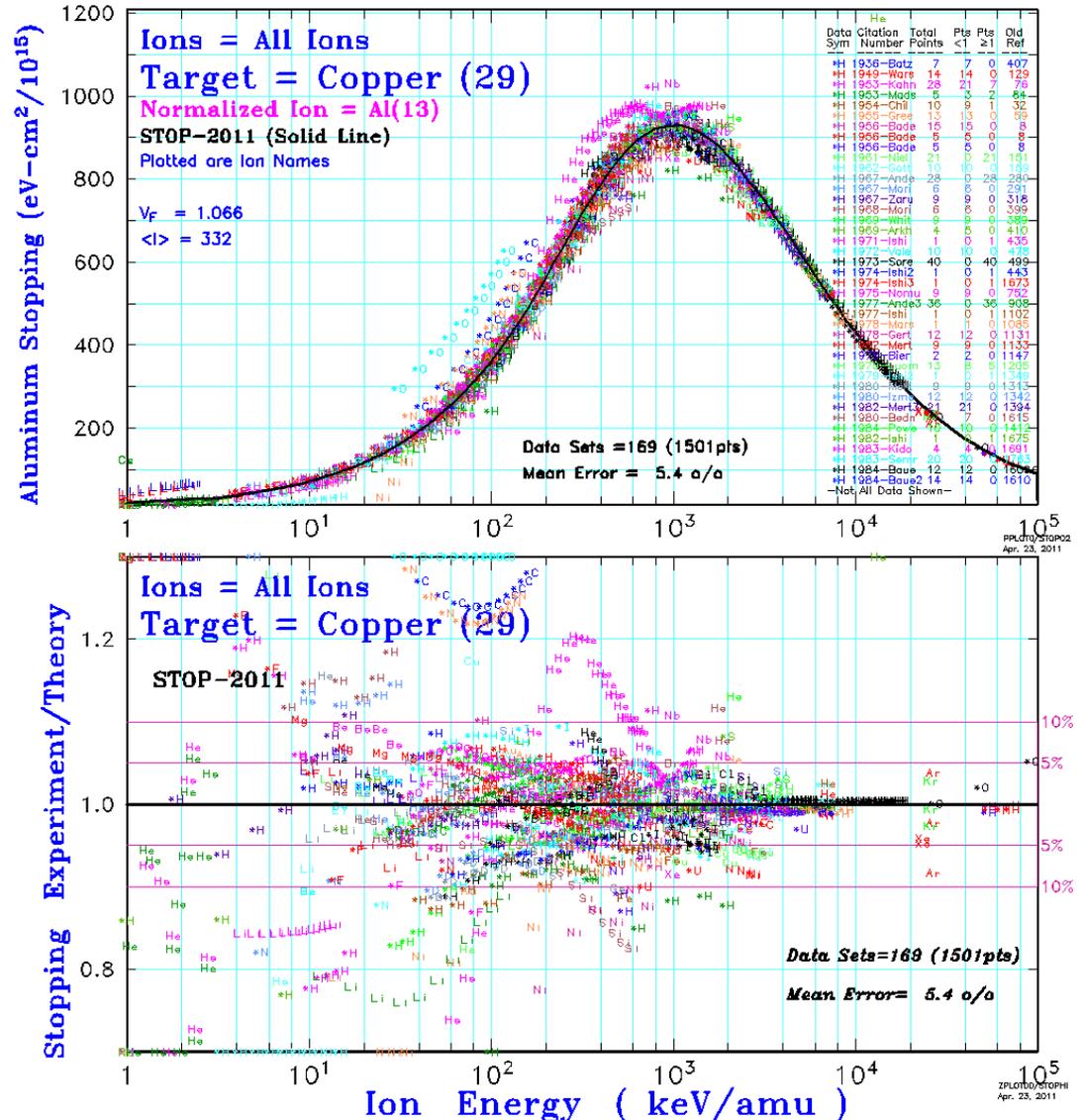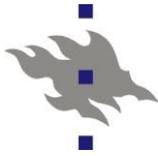
Examples of data from SRIM

■ And for

Sm

■ Just to show

not all elements

have as much data

as C and Cu
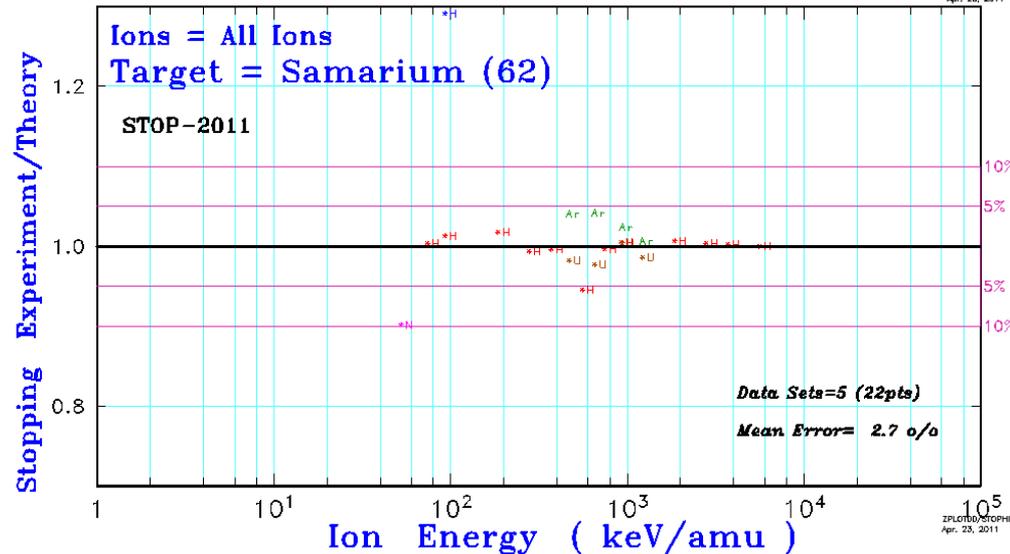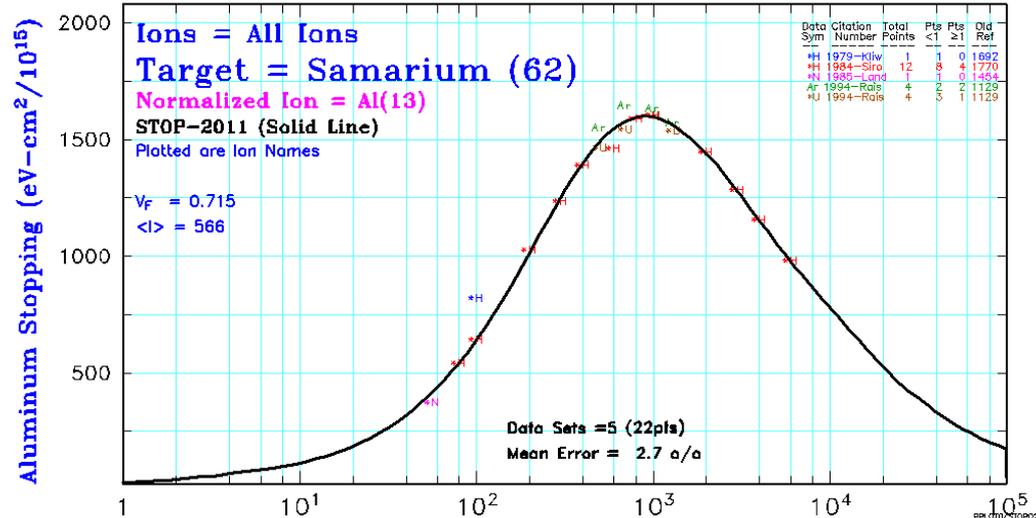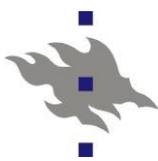
The SRIM software

- The SRIM software is freely available at the SRIM web pages
  - Often also called TRIM due to the earlier name "Transport and Range of Ions in Matter"
- It can calculate any stopping power (electronic or nuclear) in any material, including compounds and multilayer one
- It can also simulate the ion ranges based on the so called **binary collision approximation (BCA)** described later on the course
  - Includes electronic stopping in all calculations
- Downsides:
  - **Only amorphous materials modelled => no channeling**
  - It only works on Windows computers, is **not open source**, and is programmed in a quite old-fashioned way with Visual Basic
  - Because of this, installing it on modern Windows is a hassle
  - Tip: for it to work at all, one needs to set Regional settings to US English in Windows…
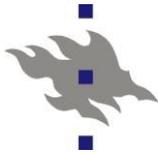
SRIM demonstration

- Step 1: select either the Stopping calculation table or "TRIM calculation"
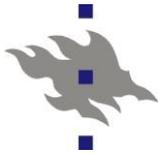
SRIM demonstration

- Setup screen for TRIM simulations
  - Select Ion Data and Target Atom element, or make a compound
  - When done, select "Save Input & Run TRIM"

Example plot of trajectories from SRIM: 200 trajectories of 10 keV protons in Si.

SRIM demonstration

- In the running window, click "Ion distribution"

Video of using SRIM

SRIM notes

- SRIM can be somewhat speeded up by closing all the output windows, and can be well ran in the background on modern multi-core processors
- Several output options exist: ion ranges, nuclear and electronic deposited energy, sputtering yield
- For detailed analyses output of file COLLISON.DAT outputs data on all ions and recoils created during the whole simulation
- **Do not use SRIM blindly: there are major caveats and pitfalls in using it, and not knowing them can lead to too much trust in accuracy of results or even outright wrong physics**
  - More on the physics behind the collisional part of SRIM later during this course
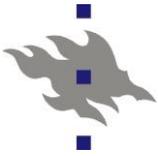
3.5. Damage from electronic stopping

- The electronic stopping does not produce damage in metals

- In ionic insulating materials it may by (at least) two mechanisms:

- 1. Single electron-excitations

  - Electrons excited by the ion can travel far from the ion path (delta electrons) and become trapped there, changing the charge state of a lattice ion

    - Since the material is an insulator, the electrons cannot travel freely to recombine with a hole

  - The changed charge state can induce a motion of the ion (as it then is in a non-equilibrium charge state) which may damage the lattice

- 2. Multiple strong excitations by swift heavy ions
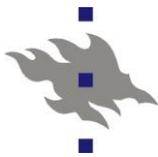
3.5.1. Single electron excitations

- The most fundamental mechanism by which electrons can cause damage is the excitation of a single chemical bond from a bonding to an antibonding state
  - This is repulsive, and hence the atoms can be pushed apart
  - Compare basic quantum mechanics, e.g. the H_2 molecules
  - Also photons can do the same thing
- Very important mechanism in molecules, organic matter
  - But poorly understood since molecules have huge numbers of possible excited bonding and antibonding states

Antibonding orbital

Bonding ground state orbital
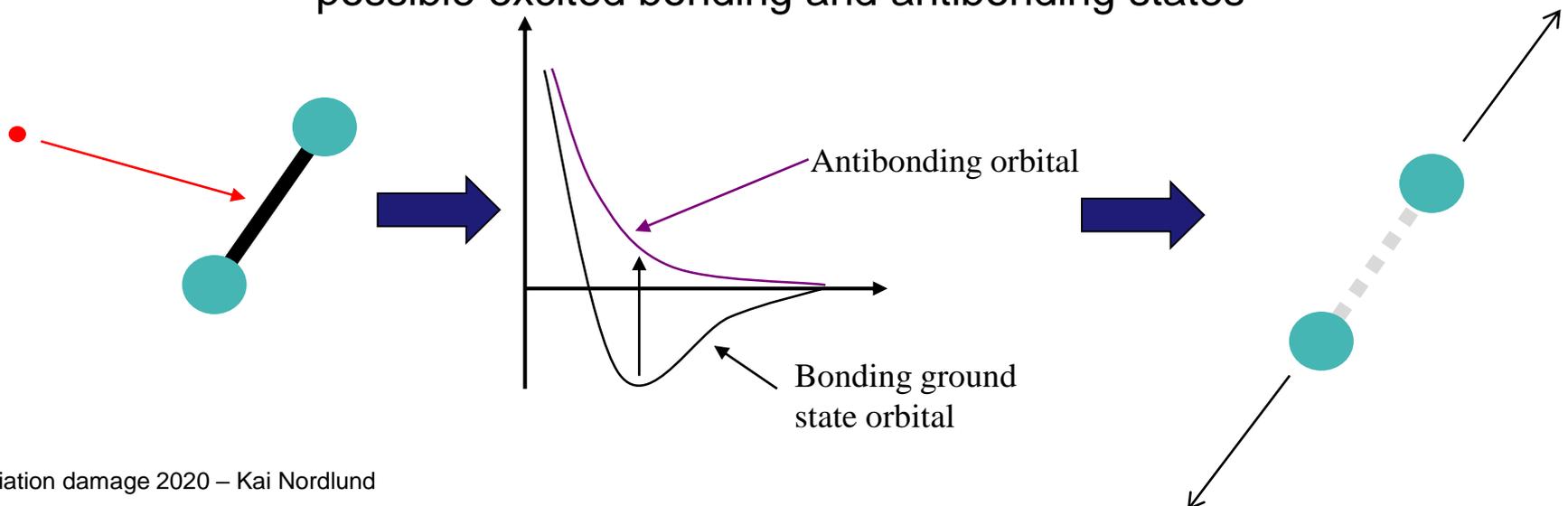
Other electronic mechanisms

- Naturally the fact that the passing ion kicks away the electrons weakens the bonds and can also put them in antibonding states
- Moreover, a heavy ion can kick out many electrons at the same time => the ion path becomes positively charged => Coulomb repulsion of positive cores, "Coulomb explosion"
  - However, it is not very clear whether Coulomb explosions really occur inside solids – neutralization may often be too rapid
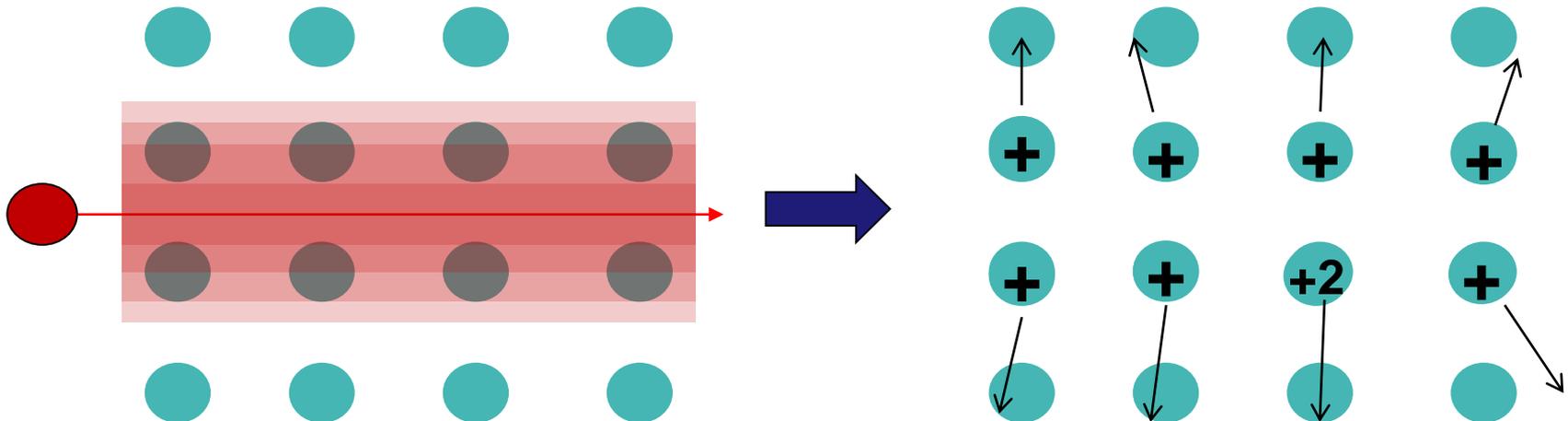
3.5.2. Swift heavy ion damage

- The swift heavy ion damage was already described to some extent in the previous section

- Reminder: it requires a high electronic stopping power, and hence has a threshold

Observed track radius vs Stopping power

~ few keV/nm

Log Stopping power vs Log Energy

~ 1 keV/amu

S_n

~ 100 keV/amu

S_e

Bragg peak (not to be confused with x-ray Bragg peaks!)
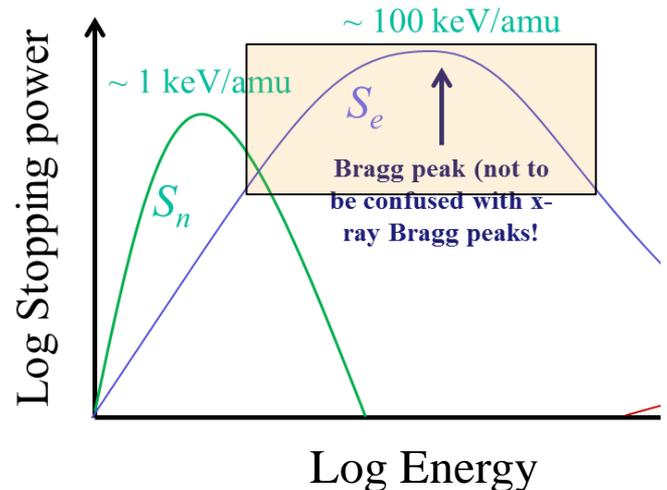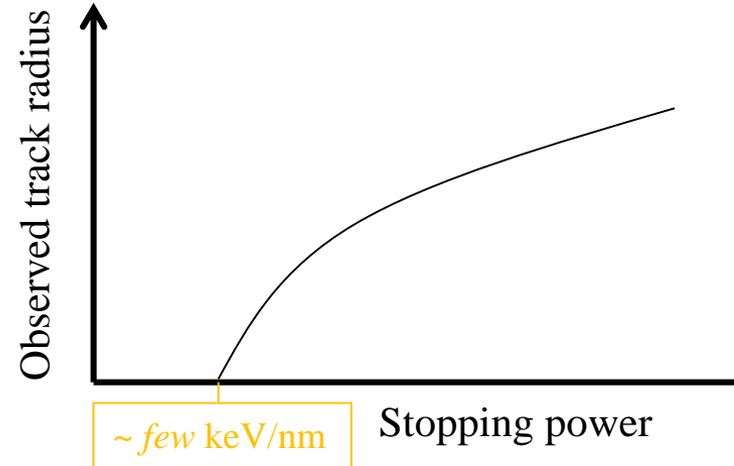
Ion path in swift heavy ion regime

■ In the swift heavy ion regime, where nuclear stopping is negligible, the ion travels essentially straight in the material

■ Near the ion path, very much electronic excitations => high electronic temperature

Au in SiO$_2$

"low energy" "high energy"

nuclear energy loss
electronic energy loss
total energy loss

~1 keV/nm

~10 keV/nm

4
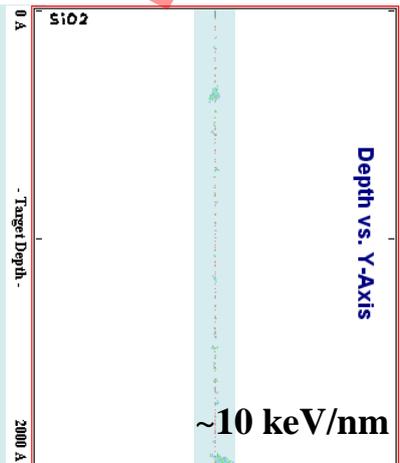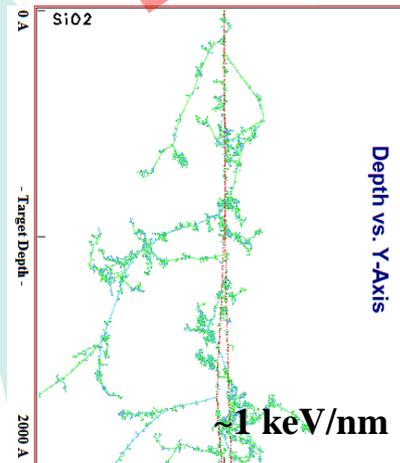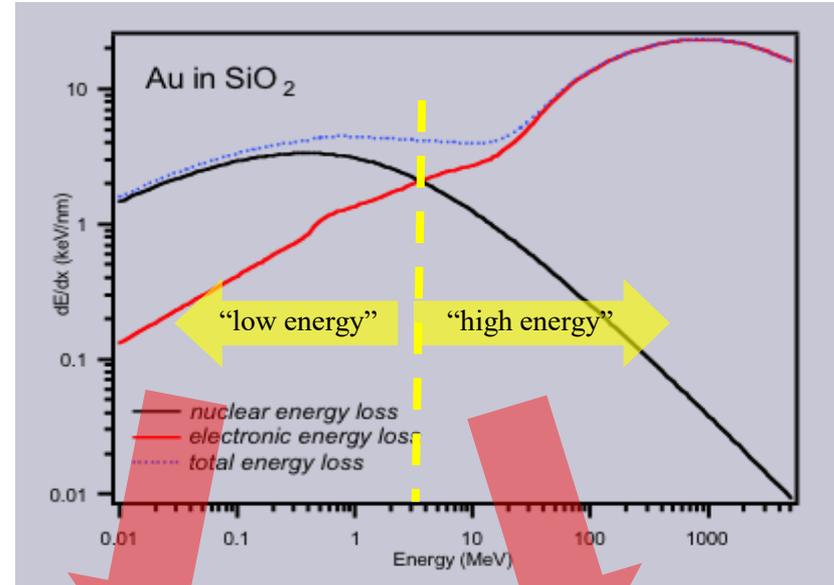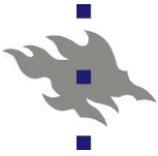
High electronic temperature

- Although the exact mechanism by which the electronic heating is not known, it appears that a two-temperature model (TTM) of lattice and electronic temperatures can be used to model it well

- Idea: swift heavy ion is the source term for the electronic system, which then via electron-phonon coupling transfers heat to the lattice (atom) subsystem)

- Same basic equations as before for EPC:

$$C_e(T_e)\frac{\partial T_e}{\partial t} = \nabla[K_e(T_e, T_l)\, \nabla\, T_e] - G(T_e)(T_e - T_l) + S(\vec{r}, t)$$

$$C_l(T_l)\frac{\partial T_l}{\partial t} = \nabla[K_l(T_l)\, \nabla\, T_l] + G(T_e)(T_e - T_l)$$
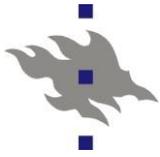
Illustration with rough time scale

■ The electronic processes occur very rapidly, < 1 ps

■ After that the lattice heating and subsequent cooling can take a much longer time

~ 0.1 fs
passage of the projectile &
initial energy deposition to electrons

~ 10 fs
electron cascade &
energy deposition to lattice

~ 1 ps
atomic motion &
restructuring
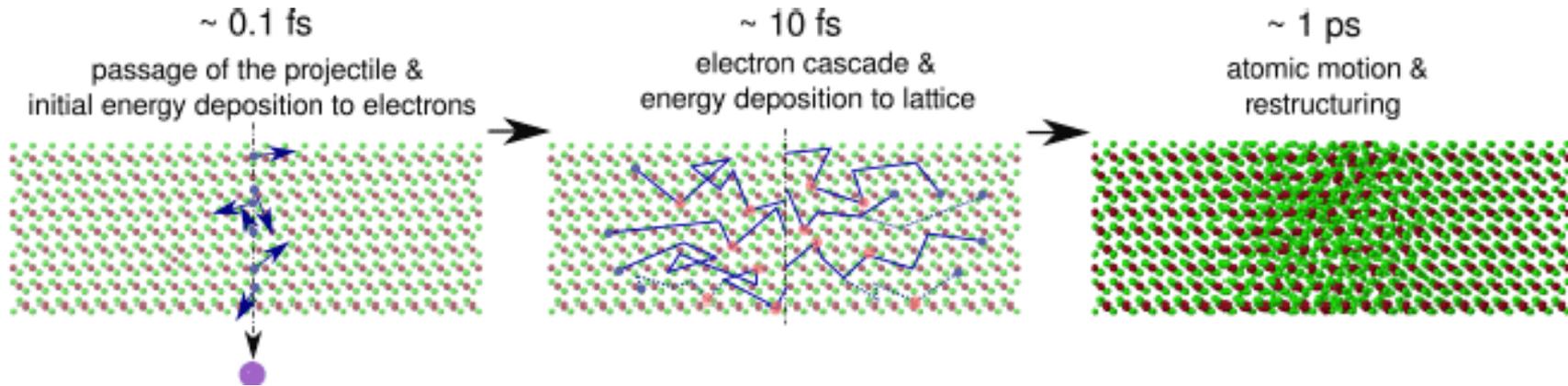
[Georg Wachter *et al* 2012 *J. Phys.: Conf. Ser.* **388** 132012]

Swift heavy ion damage

- Along the ion travel path, the material may be damaged if the lattice temperature exceeds the melting temperature
- The damage is visible as long ion tracks in a microscopy experiments
- Almost as long as ion range, can be microns easily
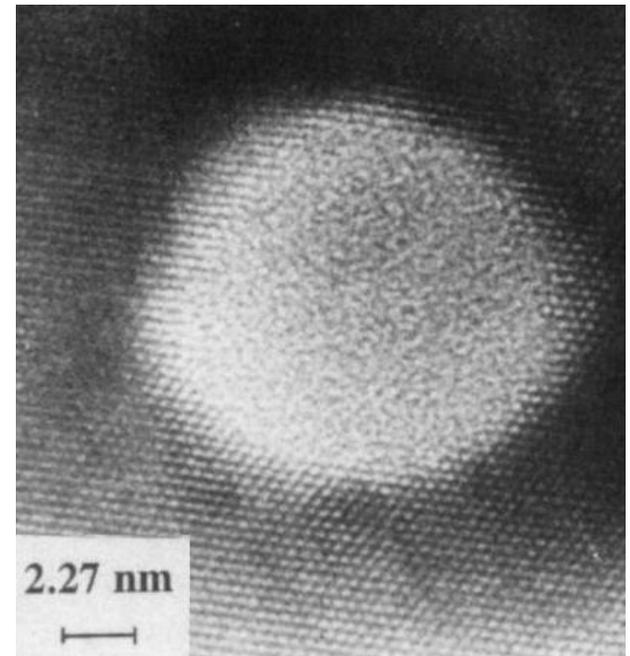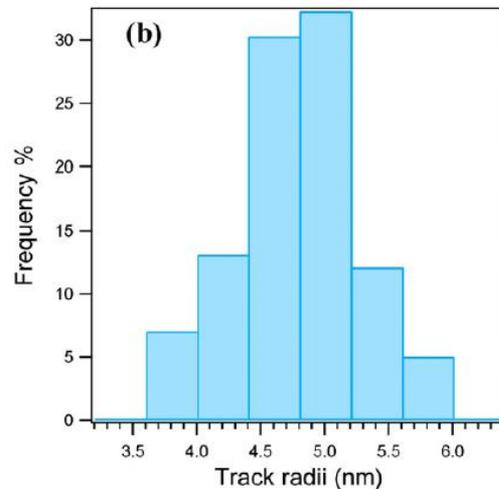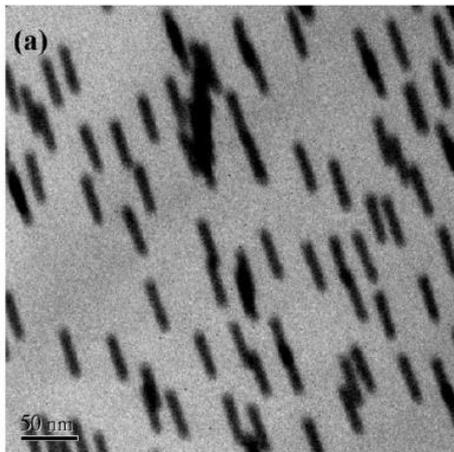
HREM experiment

A. Meftah et al. *Phys. Rev. B* **49**, 12457 (1994)

[B. Afra et al, J. Phys.: Condens. Matter 25 (2013) 045006]
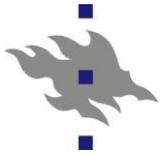
MD simulation with TTM model energy input

Ion track in quartz generated by 5.8 keV/nm energy deposition

time 0.00041 ps

x (-40 - 40) y (-30 - 30) z (-10 - 10)   Olli Pakarinen and Kai Nordlund (2008)

[Animation quartztrack2.avi]
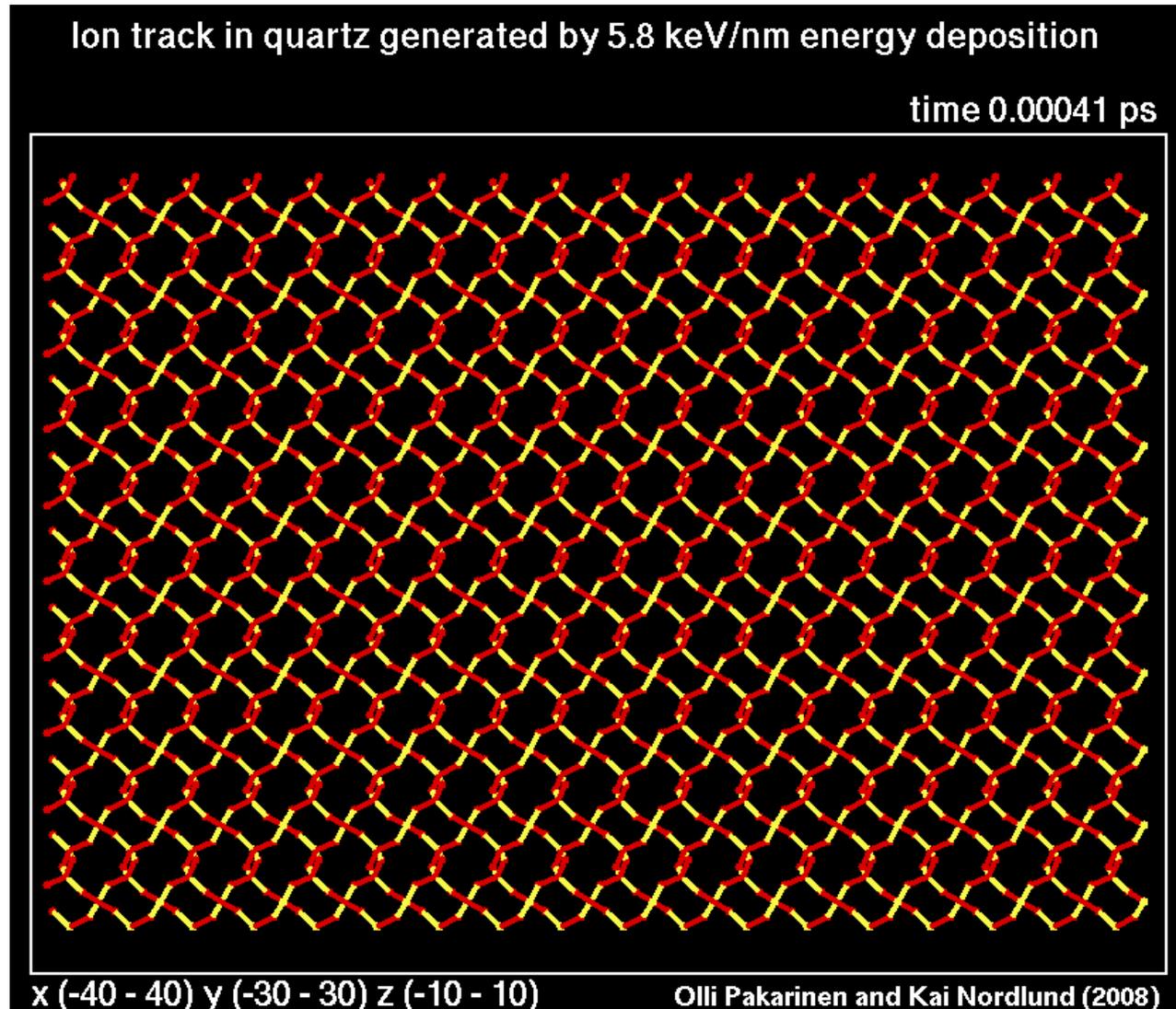
Comparison to experiments

■ The results agree well with experiments
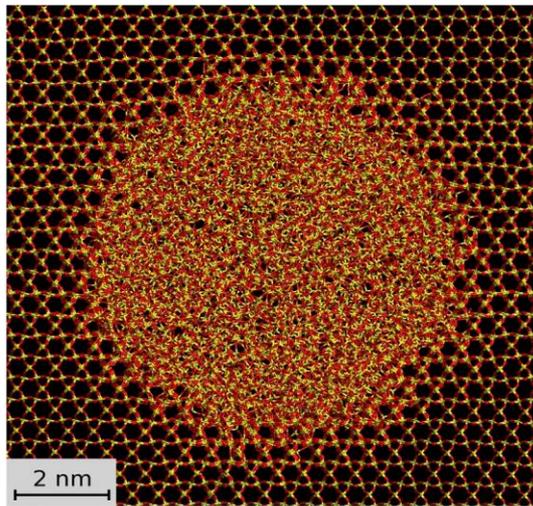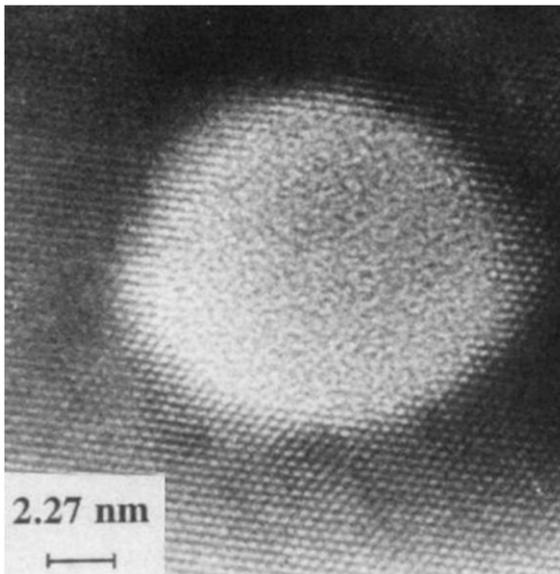
MD simulation
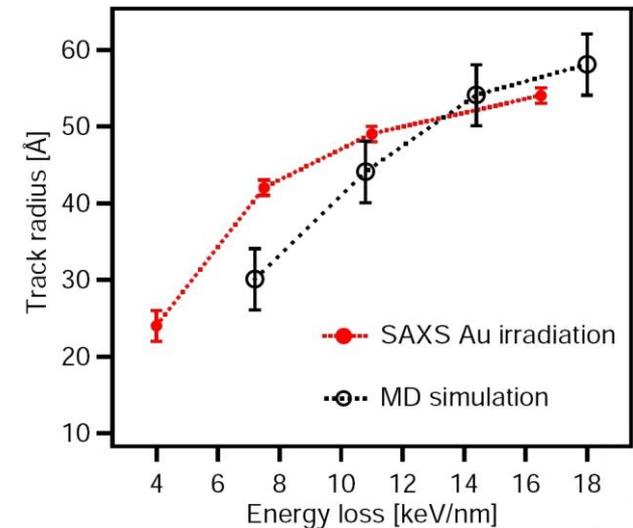
* O. H. Pakarinen, F. Djurabekova, K. Nordlund, P. Kluth and M. Ridgway, *Nucl. Instr. Meth. Phys. Res. B* 267, 1456 (2009)

Track core is underdense in some materials

■ The experiments and simulations also show that at least in some materials, the track core is actually underdense
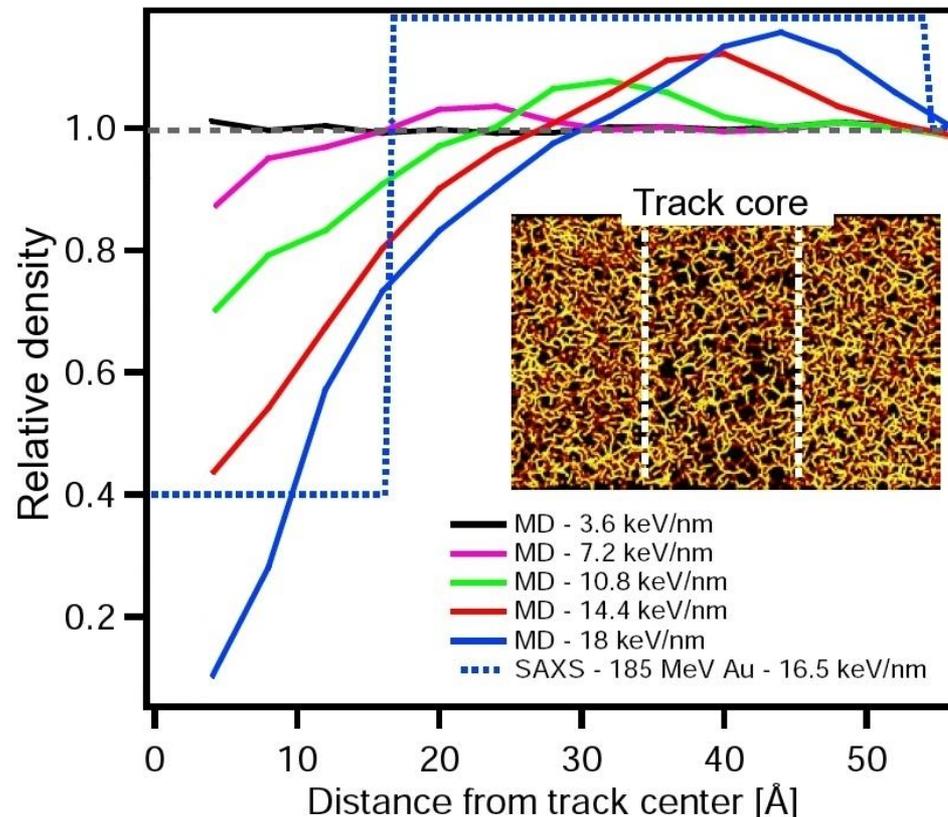
* O. H. Pakarinen, F. Djurabekova, K. Nordlund, P. Kluth and M. Ridgway, *Nucl. Instr. Meth. Phys. Res. B* 267, 1456 (2009)

Applications of ion tracks, 1

- The ion tracks have actually industrial applications
- Since the track core has a different structure from the surrounding material, it may be etched away with a suitable chemical that affects only the disordered region
- This can leave a pore behind => one can make nanoporous filters
- Already a standard technique for polymer foils
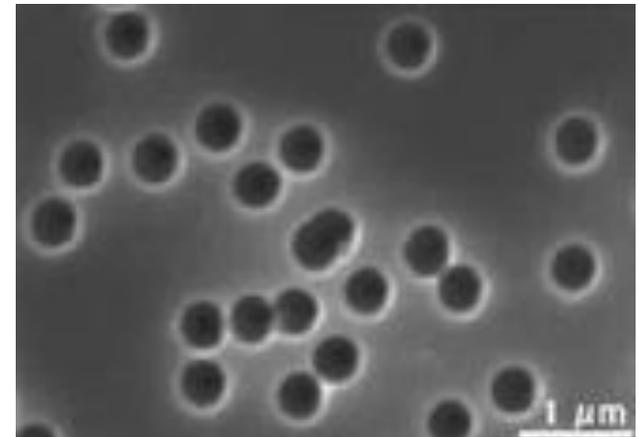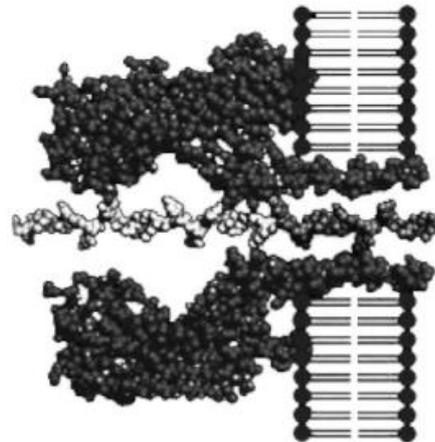
R. Spohr, Radiation Measurements (2005)

[More recent review: Maria E. Toimil-Molares, Beilstein Journal of Nanotechnology 3 (2012) 860.

Applications of ion tracks, 2

- **The ion track irradiation can also be used as a tool in lithography**
  - Since they travel in long straight paths, they can make high-aspect ratio structures in materials
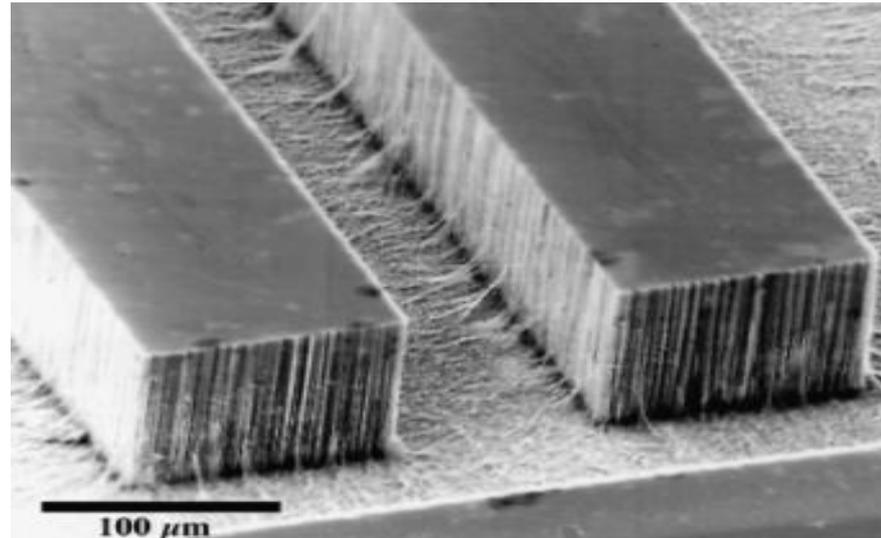
G. Thornell *et al.* Sensors and Actuators (1999)

What should you have learned from this section?

- You understand the physical origin of electronic stopping power at all experimentally accessible energies

- You know the basic range concepts

- You understand ion channeling in crystalline materials

- You know about SRIM and the basics of how to use the code

- You know about swift heavy ion tracks and the basics of how they are created