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Radiation Damage in Materials

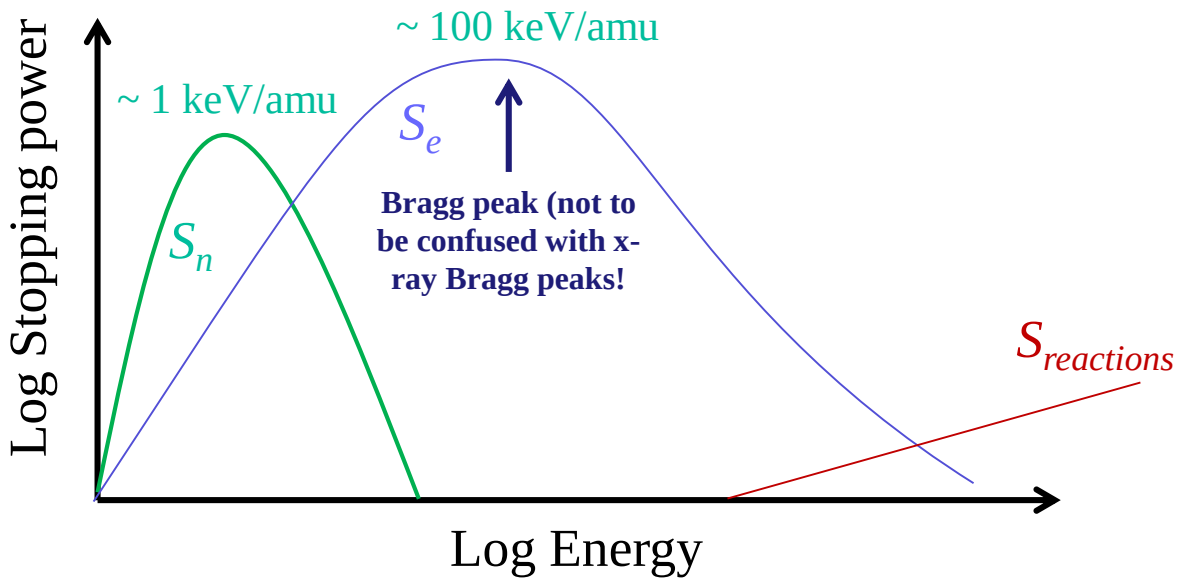
4. Nuclear stopping and atomic collisions

[Section contents mainly by Prof. Flyura Djurabekova]

4.1. Physical origin of nuclear stopping power

- Recall from previous section the definition of stopping power

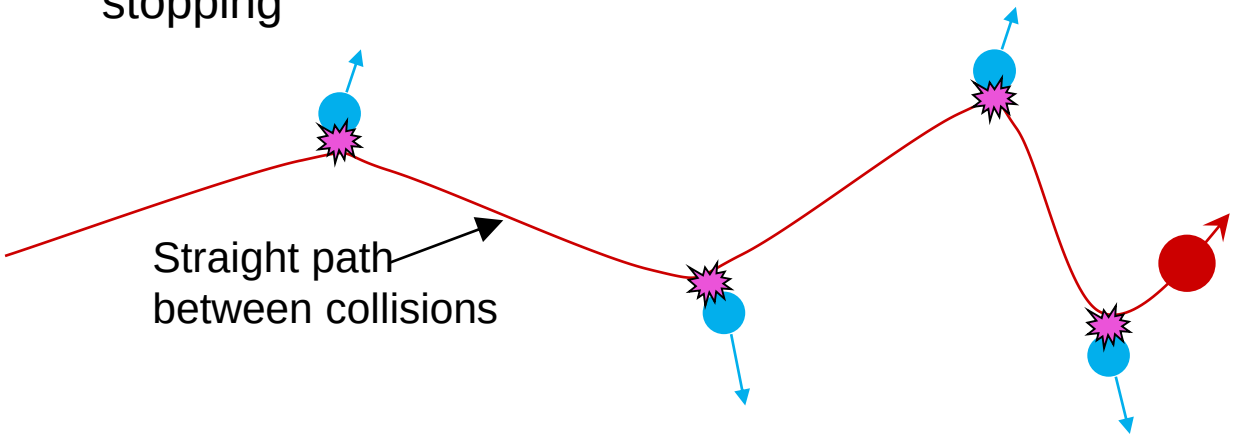
$$S = -\frac{dE}{dx} = S_n + S_e + S_{reactions}$$



- Now we will consider the nuclear stopping power in more detail, especially its physical origins

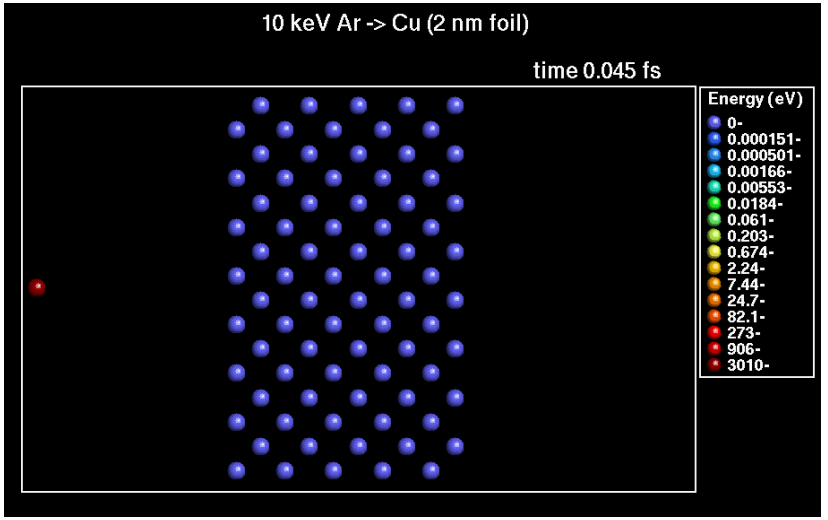
Nuclear stopping power from collisions

- When an ion/recoils moves in a lattice, it collides with the atoms in it
- In each collision, it transfers some momentum and energy to the lattice atom => energy loss => nuclear stopping
  - If the collision cross section is low, it collides only occasionally, and moves straight in between
    - All the time it loses energy also to electrons via electronic stopping

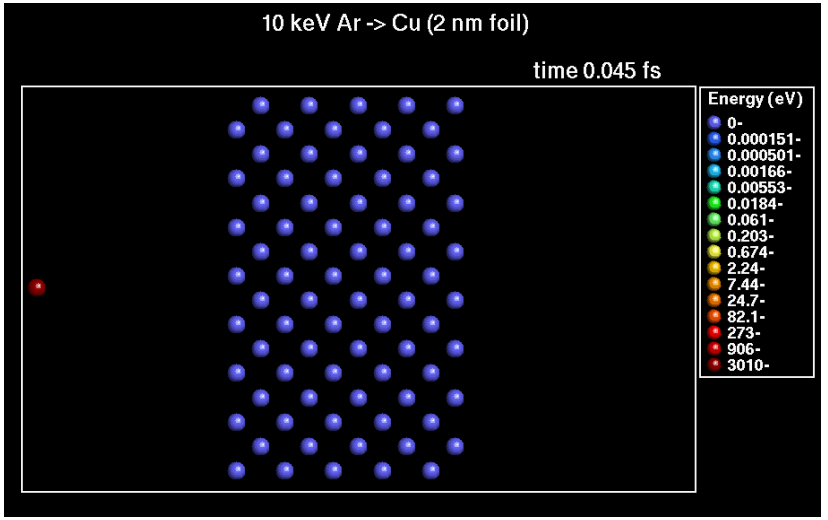


Multiple vs. single collisions

- Animations of the difference between single and multiple collisions:
  - 10 keV Ar -> Cu very thin foil (2 nm)
- Upper part: all atom movements taken into account
- Lower part: strongest binary collisions only



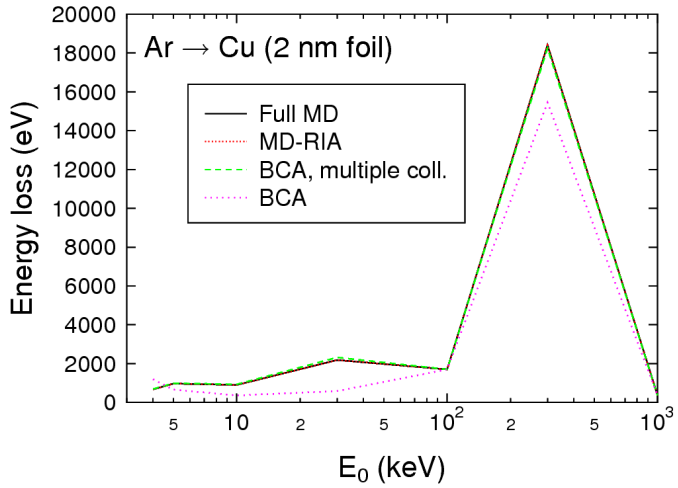
[Animation: 10kevar_cu2nm.avi]



[Animation: 10kevar_cu2nm_bca.avi]

Energy loss

- The nuclear stopping power S_n(E) is simply the average energy loss per unit path length travelled from all the collisions
- In principle it is always from all the multiple simultaneous collisions
- But for high ion/recoil energies >> 1 keV, the collision cross section becomes low, and a few binary collisions tend to dominate the energy loss
- For the example case of Ar -> Cu, for $E \geq 1\,00\ \mathrm{keV}$, single binary collision model very accurate



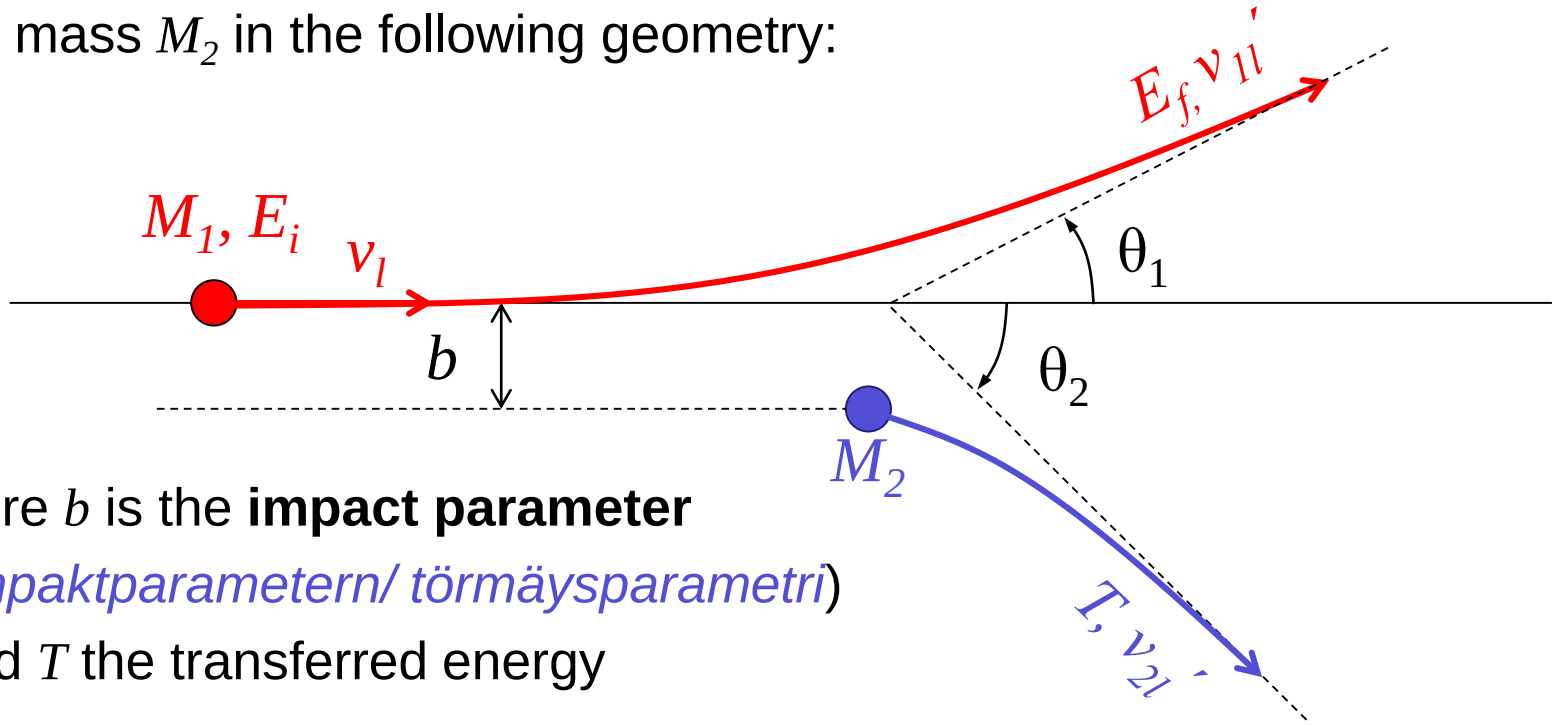
[K. Nordlund, NIM B 266 (2008) 1886]

Independence of nuclear and electronic stopping

- A natural question is whether the nuclear and electronic stopping depend on each other
  - For instance, since a strong collision will likely also excite electrons of the atom, one might think that high nuclear stopping enhances the electronic one
- However, a wide range of theoretical and experimental studies indicate the two effects are almost completely independent of each other for stopping and damage production
  - Very recent work shows that there is a small energy range where nuclear and electronic processes contribute both to the stopping and damage, but this is a rather marginal effect and seldom important [Debelle et al, Phys. Rev. B 86 (2012) 100102]

4.2. The binary collision scattering integral

- Since the **binary collision (***binärkollision/binääritörmäys***)** dominates nuclear stopping power, we treat it here in mathematical detail
- The basic premise is the following: a moving atom with velocity v_l of mass M_1 and initial energy E_i is impacting on an atom at rest of mass M_2 in the following geometry:

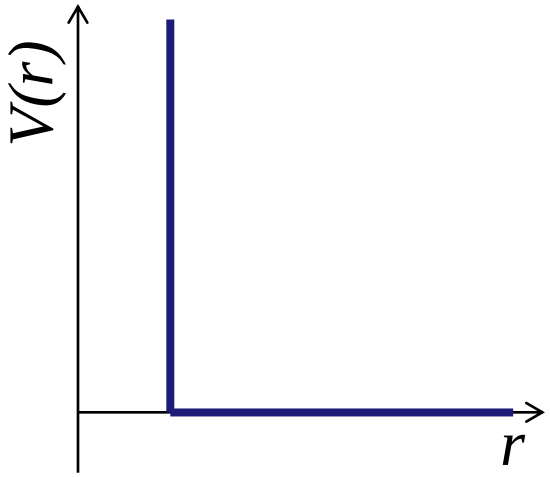


- Here b is the **impact parameter** (*impaktparametern/ törmäysparametri*) and T the transferred energy

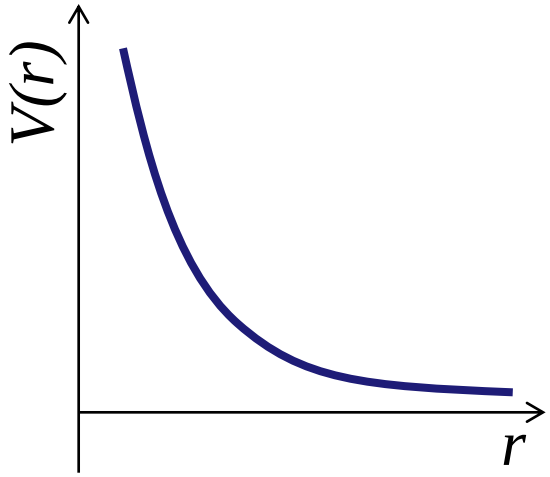
Central-force scattering

- The binary collision movement can be solved analytically provided the interatomic interaction is a so called central force one, i.e. depends only on the interatomic distance: $V = V(r)$
- The problem is actually quite general, and applies to also classical atom-nucleus, atom-electron etc. collisions.
- The potential can in principle be any function that only depends on r, but the following three types are important:

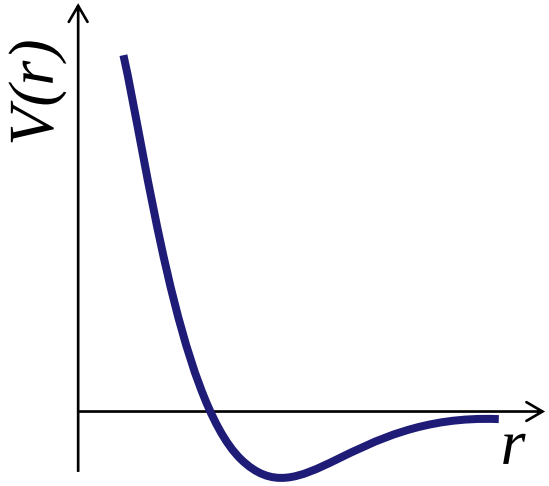
Hard-sphere potential



Purely repulsive potential

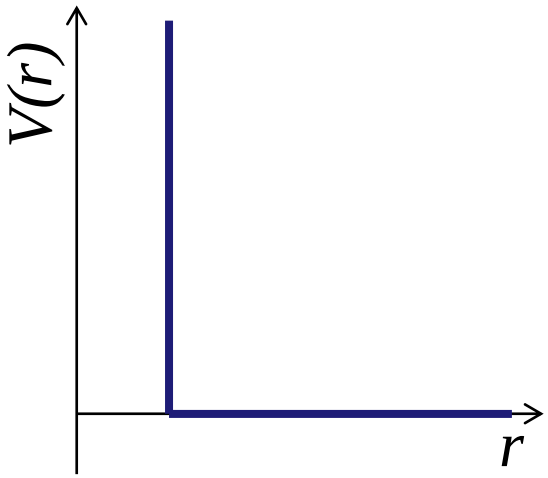


Potential with attractive well

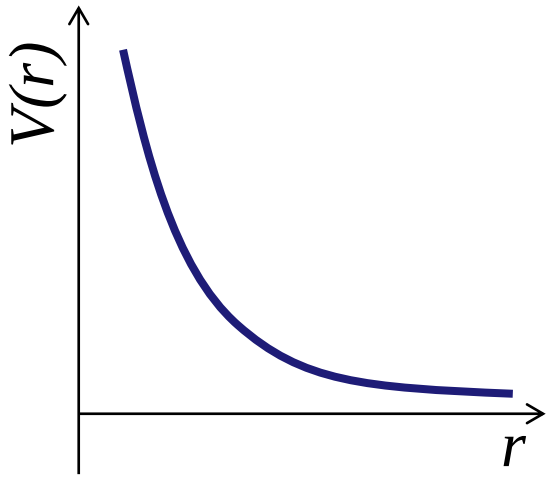


Where are they important?

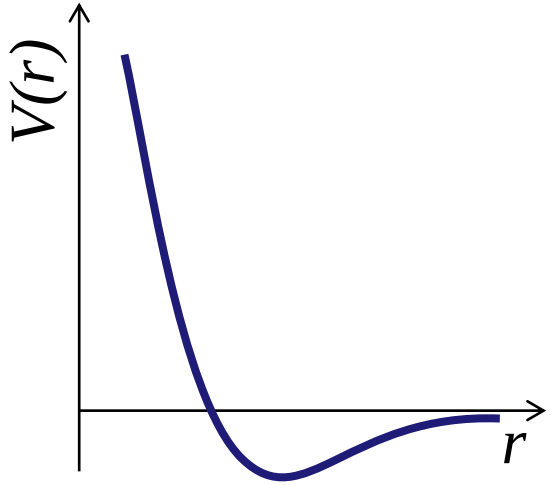
1. Hard-sphere potential



2. Purely repulsive potential



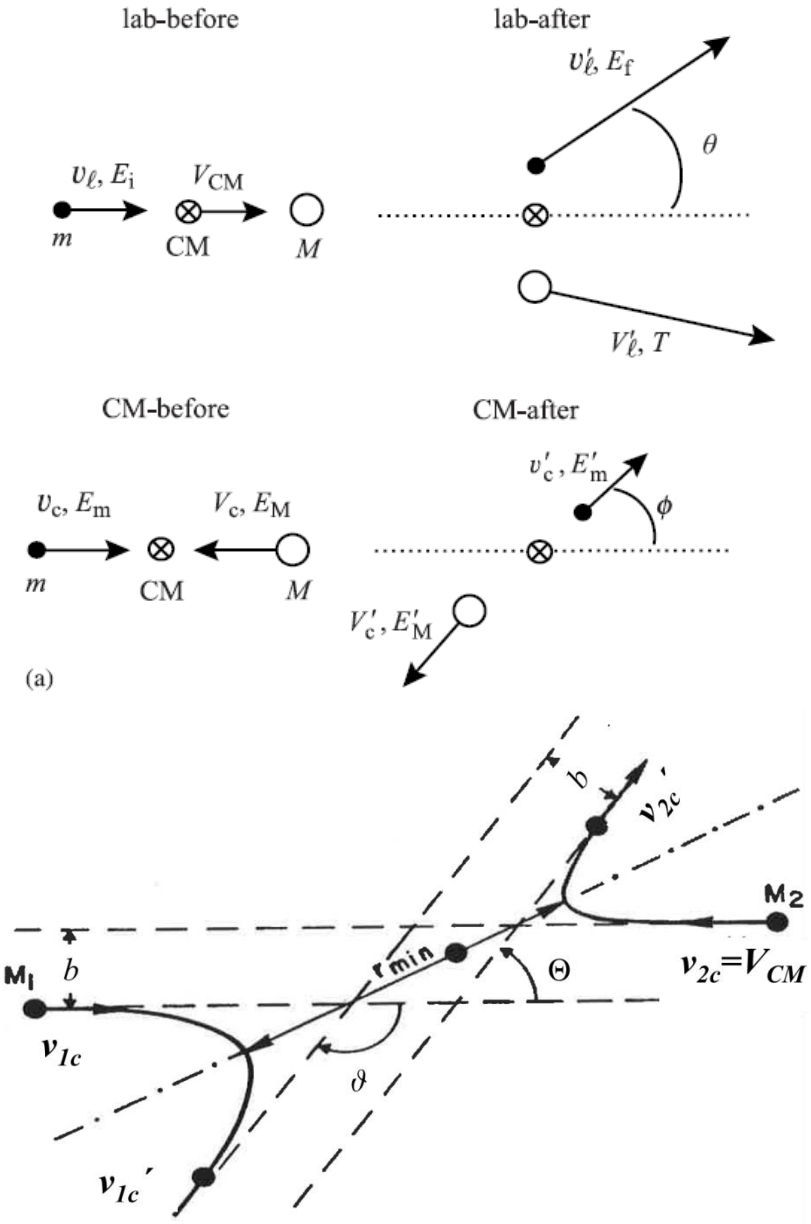
3. Potential with attractive well



1. The simplified type 1 is actually quite good for describing elastic atom-nucleus collisions (nucleus is small and ‘hard’)
2. Any collision between charged particles of the same charge leads to a purely repulsive (Coulomb) potential.
   - If it is two nuclei, this is known as **Rutherford scattering** (*spridning/sironta*)
3. The interaction between two neutral atoms has an attractive well due to chemical (covalent, metallic, van der Waals) effects

Center-of-mass (CM) coordinates

- To simplify the problem, we will consider the collision of two particles in 2D geometry, in the plane where the collision is held.
- To solve the two-body collisional process, it is useful to go via Center-of-Mass coordinates instead of lab coordinates (LC)
  - In these the CM does not move
- Why is it needed? Because atoms “move” along one line as in simple face-to-face collisions
  - Before the collision towards one another
  - After the collision in opposite directions.
- We know how CM moves in LC, hence the results obtained in CM can be converted back in LC



Velocities in CM before and after collision

- We will consider a collision of two particles moving in CM
  - a projectile with mass m and velocity in CM v_{1c} (v_{1c}' after the collision)
  - a target particle with mass M and velocity in CM v_{2c} (v_{2c}' after the collision).
- The total momentum of such system will be zero. Momentum conservation gives us that

$$\begin{aligned} v_{1c}M_1 - v_{2c}M_2 &= 0 \\ v'_{1c}M_1 - v'_{2c}M_2 &= 0 \end{aligned} \qquad (1)$$

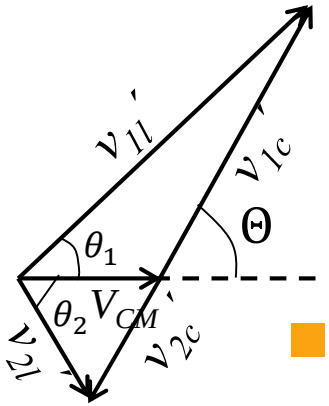
- Energy conservation then

$$\frac{1}{2}M_1 v_c^2 + \frac{1}{2}M_2 v_{2c}^2 = \frac{1}{2}M_1 v_{1c}'^2 + \frac{1}{2}M_2 v_{2c}'^2 \qquad (2)$$

- Combine (1) and (2) together and it will be obvious that velocities in CM before and after collision do not change their absolute value $\left(\frac{1}{2}M_1\left(\frac{M_2}{M_1}\right)^2 + \frac{1}{2}M_2\right)v_{2c}^2 = \left(\frac{1}{2}M_1\left(\frac{M_2}{M_1}\right)^2 + \frac{1}{2}M_2\right)v_{2c}'^2$

Recoil velocity in LC

- Velocity in the LC will be calculated as $\vec{v}_l = \vec{v}_c + \vec{V}_{CM}$
- Since both particle and CM move in the same direction then the relation of CM velocity to LC velocity is $v_{1c} = v_{1l} - V_{CM}$
- The target particle (not moving in LC) moves in CM with the same velocity (opposite sign only) as the CM itself in LC, or $v_{2c} = -V_{CM}$.
- Using these in (1) we find that $V_{CM} = \frac{M_1}{M_1 + M_2} v_{1l}$ (3)
- After the collision, target particle will receive some recoil energy ***T*** and move with corresponding recoil velocity V'_l. Applying the cosine rule to sum the vectors:



$$\vec{v}'_{2l} = \vec{v}'_{2c} + \vec{V}_{CM} \rightarrow v'^2_{2l} = v'^2_{2c} + V^2_{CM} - 2v'_{2c}V_{CM}\cos\Theta = 2V^2_{CM}(1-\cos\Theta)$$

- since $\left|\vec{V}_{CM}\right| = \left|\vec{v}_{2c}'\right|$. Here Θ is scattering angle in CM, which is related to the scattering angle in LC θ_2 (see figure) as

$$\theta_2 = (\pi - \Theta)/2 \qquad (4)$$

Recoil energy (energy transferred in collision)

- Now we apply (3) and (4) and finally obtain

$$v_{2l}'^2 = 2V_{CM}^2(1-\cos\Theta) = 2V_{CM}^2(1-\cos(\pi-2\theta_2)) =$$

$$2V_{CM}^2(1+\cos 2\theta_2) = 2V_{CM}^2(1+(2\cos^2\theta_2-1)) = 4\frac{M_1^{\,2}}{(M_1+M_2)^2}v_{1l}\cos^2\theta_2$$

- The recoil velocity in LC then is

$$v_{2l}' = \frac{2M_1}{(M_1+M_2)}v_{1l}\cos\theta_2$$

- This gives us also transferred in collision energy, which is

$$T = \frac{1}{2}M_2 v_{2l}'^2 = \frac{4M_1^{\,2}M_2}{2(M_1+M_2)^2}v_l^2\cos^2\theta_2 = 4\frac{M_1M_2}{(M_1+M_2)^2}E_i\cos^2\theta_2$$

- This equation gives us a clear idea that the maximum energy will be transferred in face-to-face collision ($\theta_2 = \pi$)

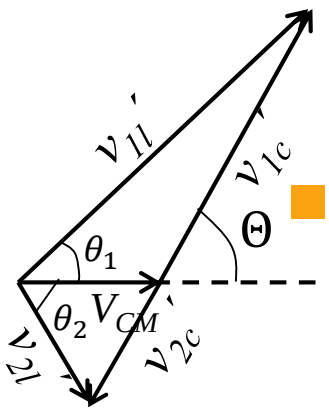
Scattering angles in LC

- Even if now we know how to find the transferred energy, it is still not clear how to find the angle θ_1.
- In general, to describe the collision fully we need to know both scattering angles (for projectile and target particle) in LC.
- Let's look again in this figure, and remembering Eq.(1) that

$$v'_{1c} = -\frac{M_2}{M_1} v'_{2c} = \frac{M_2}{M_1} V_{CM}$$

- We find

$$\tan\theta_1 = \frac{v'_{1c}\sin\Theta}{V_{CM} + v'_{1c}\cos\Theta} = \frac{\frac{M_2}{M_1}\sin\Theta}{(1+\frac{M_2}{M_1})\cos\Theta} = \frac{M_2\sin\Theta}{M_1 + M_2\cos\Theta}$$



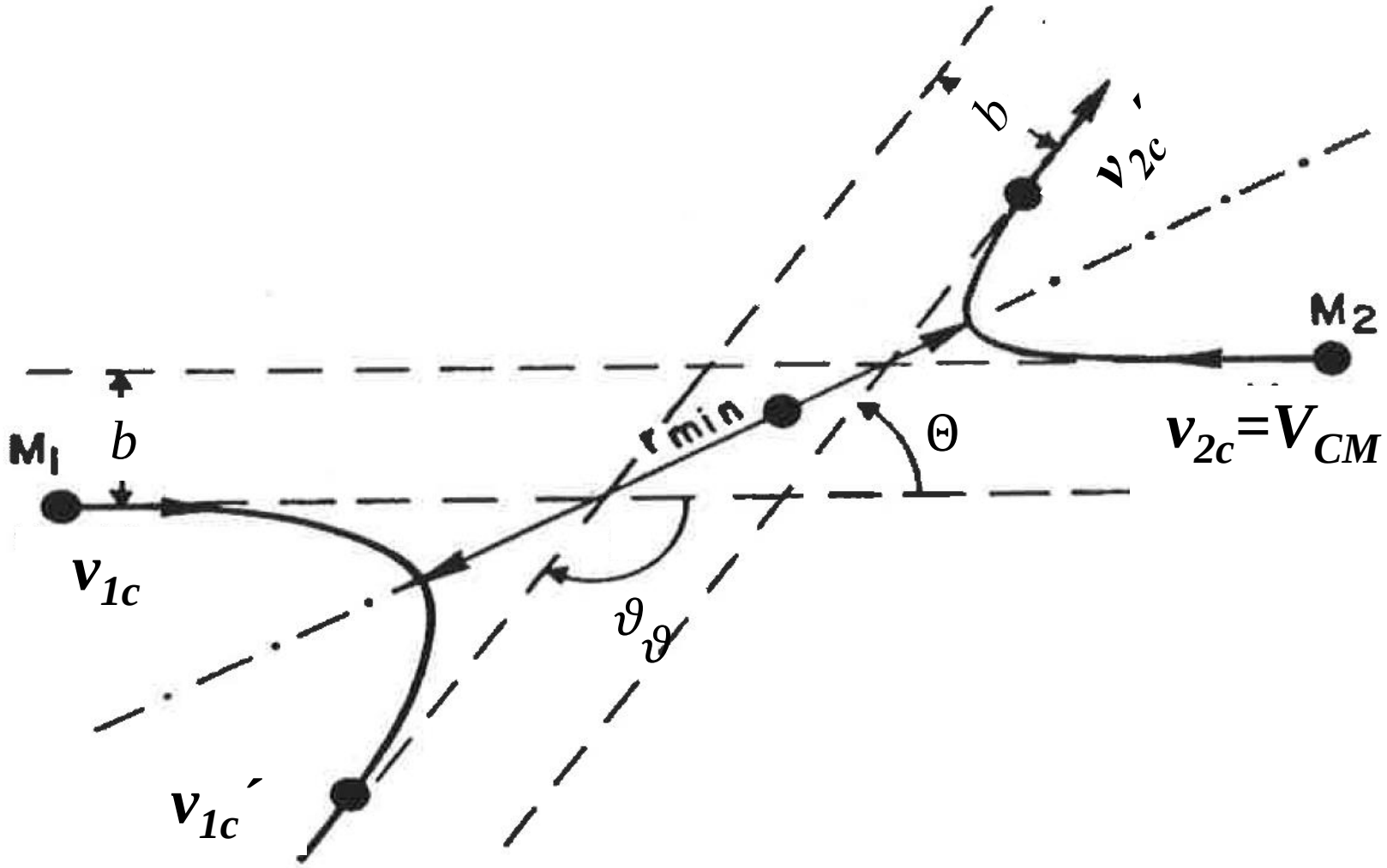
- And finally we can say that we know that the scattering angles in LC (angles in the plane of the collision) of both particles relate to a single scattering angle in CM as

$$\theta_2 = \frac{\pi - \Theta}{2}; \quad \tan\theta_1 = \frac{M_2\sin\Theta}{M_1 + M_2\cos\Theta} \qquad (5)$$

The two-body scattering integral solution

- However, we need to know this angle Θ and for this we need to solve the scattering integral!
- All what we have to do is to find the trajectories of particles in CM.
  - As was said before, the problem is two-dimensional and belongs in the plane formed by the vector of initial velocity and the initial position of the target particle.
- The problem can be solved easier if we remember about polar coordinates. This polar coordination system will be associated with CM, since the motion of both particles in CM is symmetric and linear momentum before and after collision is zero.
  - We will need two polar ϑ and radial r coordinates (illustration is given in the next slide).
- The motion can be considered in the potential field $V(r)$ centered at the center of mass.

Illustration of motion of two colliding particles in CM



Derivation of integral of motion

- Energy conservation demands that the energy, initially available in the system (in CM) remains constant, or

$$E_{CM} = \frac{1}{2} M_c \left(\frac{dr}{dt}^2 + r^2 \frac{d\vartheta}{dt}^2 \right) + V(r) \qquad (6)$$

- Here E_{CM} and M_C are the energy and reduced mass in CM

$$\left(E_{CM} = \frac{1}{2}\left(M_1 v_{1c}^{\ 2} + M_2 v_{2c}^{\ 2}\right) = \frac{1}{2}\left(M_1 \left(\frac{M_2}{M_1}\right)^2 + M_2 \right) V_{CM}^{\ 2} = \frac{1}{2}\frac{M_1 M_2}{M_1 + M_2} v_{1l}^2 = \frac{M_c v_{1l}^2}{2} \right)$$

- Also, the angular momentum $J_C = M_C r^2 \frac{d\vartheta}{dt}$ is also conserved and is defined by the impact parameter b and the initial velocity of the system $J_C = M_C v_{1l} b$, which gives us $\frac{d\vartheta}{dt} = \frac{v_{1l} b}{r^2}$ (7)
- then we can re-write Eq. (6) as radial equation of motion

$$E_{CM} = \frac{1}{2} M_c \left(\left(\frac{dr}{dt} \right)^2 + r^2 \left(\frac{b v_{1l}}{r^2} \right)^2 \right) + V(r) \rightarrow 1 = \frac{1}{v_{1l}^2} \left(\left(\frac{dr}{dt} \right)^2 + \frac{b^2}{r^2} \right) + \frac{V(r)}{E_{CM}}$$

- Finally we obtain $$\frac{dr}{dt} = v_{1l}\sqrt{1-\frac{b^2}{r^2}-\frac{V(r)}{E_{CM}}} \qquad (8)$$
- Integrating this can give the time evolving trajectory in CM, which needs extra efforts to convert it in LC
- In many cases it is enough to find the azimuthal angle of scattering, which can be easily converted in LC angles as we saw in Eq.(5). Then, combining (7) and (8) we will have

$$\frac{d\vartheta}{dr} = \frac{d\vartheta}{dt}\frac{dt}{dr} = \frac{v_{1l}b}{r^2 v_{1l}\sqrt{1-\frac{b^2}{r^2}-\frac{V(r)}{E_{CM}}}} = \frac{b}{r^2\sqrt{1-\frac{b^2}{r^2}-\frac{V(r)}{E_{CM}}}}$$

- Now we need only to integrate this expression over all range of r $-\infty$ to $+\infty$

Scattering angle in CM (integral of motion)

- The maximum deflection angle in CM (following the polar coordinate direction in illustration in slide 16) is

$$\vartheta = \int_{-\infty}^{+\infty} \frac{bdr}{r^2\sqrt{1-\frac{b^2}{r^2}-\frac{V(r)}{E_{CM}}}}$$

- Now, from the same illustration we see that the angle Θ is related to the angle ϑ as $\Theta = \pi - \vartheta$.
- Then, finally

$$\Theta = \pi - \int_{-\infty}^{+\infty} \frac{bdr}{r^2\sqrt{1-\frac{b^2}{r^2}-\frac{V(r)}{E_{CM}}}} = \pi - 2\int_{r_{\min}}^{+\infty} \frac{bdr}{r^2\sqrt{1-\frac{b^2}{r^2}-\frac{V(r)}{E_{CM}}}}$$

From solution to scattering cross section

[Was, p.30; Smith, pp.36-38]

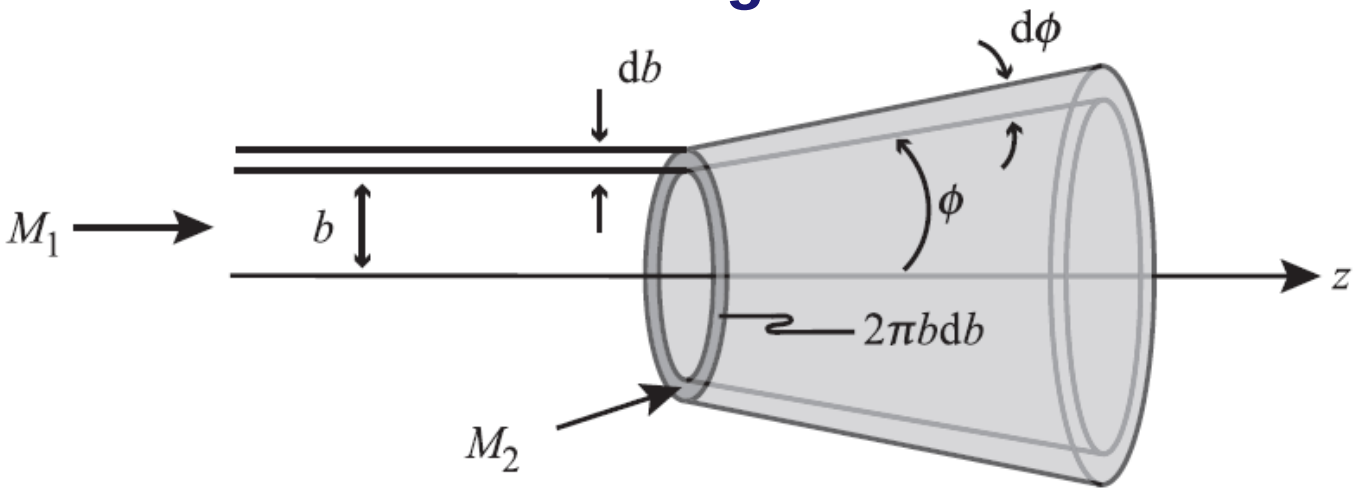
- We saw how we can calculate the energy transferred in collision, which can be considered as a energy loss.
- Is it possible to estimate these losses as a continuous function?
- The answer is “yes”. And this is the nuclear stopping power defined in section 3, which is known as the amount of energy lost on nuclear collisions per unit length and denoted as

$$S_n(E) = -\frac{dE}{dx}\frac{1}{N}$$

where N is the atomic density

- This interpretation is convenient as it gives general understanding of when and why a projectile will stop in the matrix.

Cross section of scattering

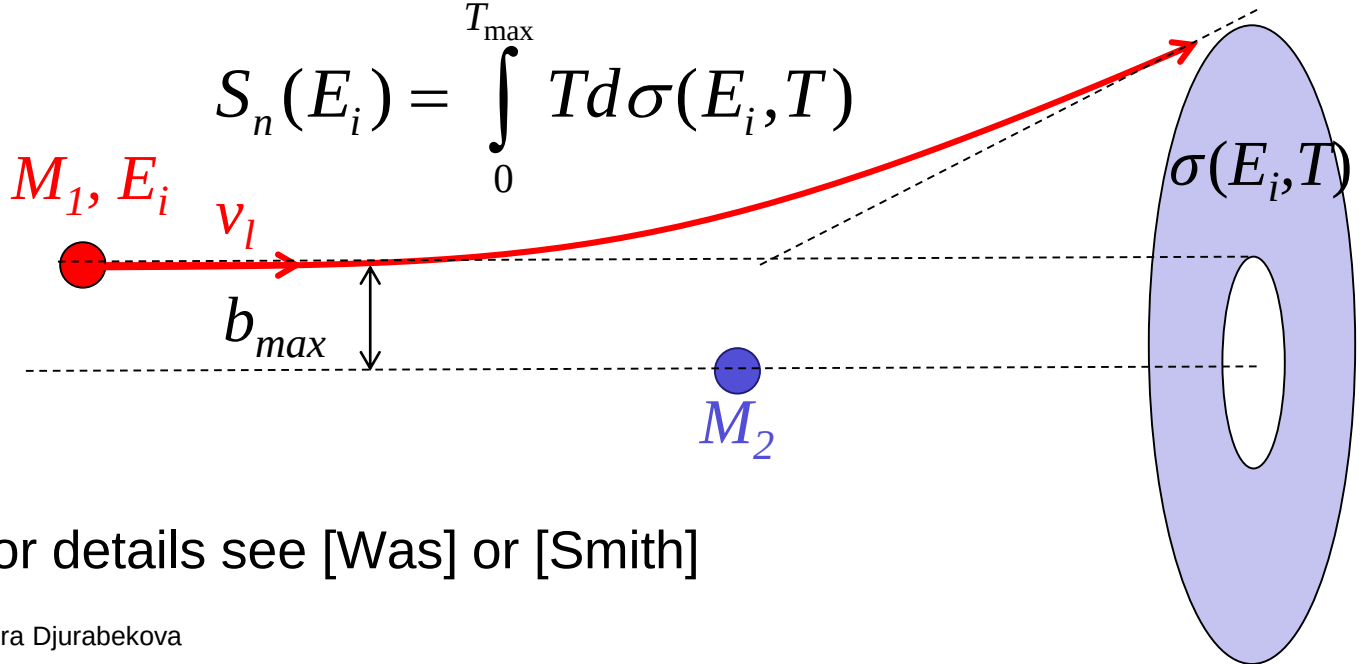


- Generally speaking we can consider a number of particles which will collide with target atoms with the impact parameters $b \pm db$ (all particles within the cross-section $2\pi b db$)
- These particles will scatter within the solid angle interval $d\phi$, which depends on initial energy E_i and transferred energy T for given pair of atoms.
- The scattering cross-section can be found as $d\sigma(E_i, T) = -2\pi \frac{db}{d\phi} d\phi$

Nuclear stopping power

- Integrating the last expression over all impact parameters b (from zero to the b_{max}) and all the transferred energies on what the scattering angle also depends, will give us a functional form for total cross section of scattering, which can be used to calculate the stopping power.

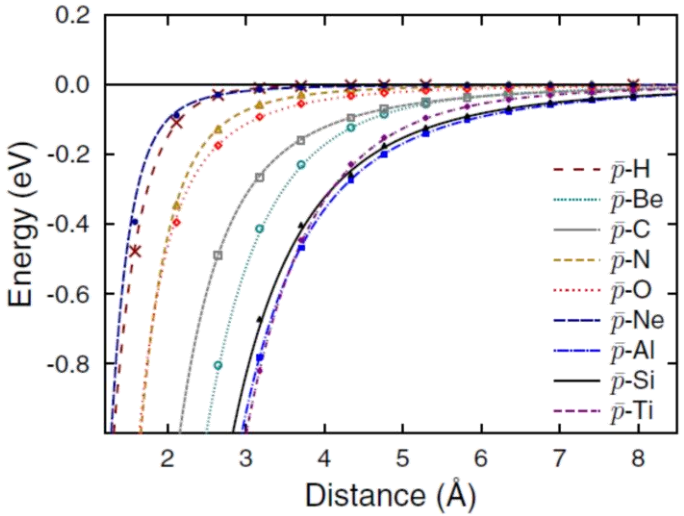
$$S_n(E_i) = \int_0^{T_{\max}} T d\sigma(E_i, T)$$



- For details see [Was] or [Smith]

A special case: nuclear stopping power of antiprotons

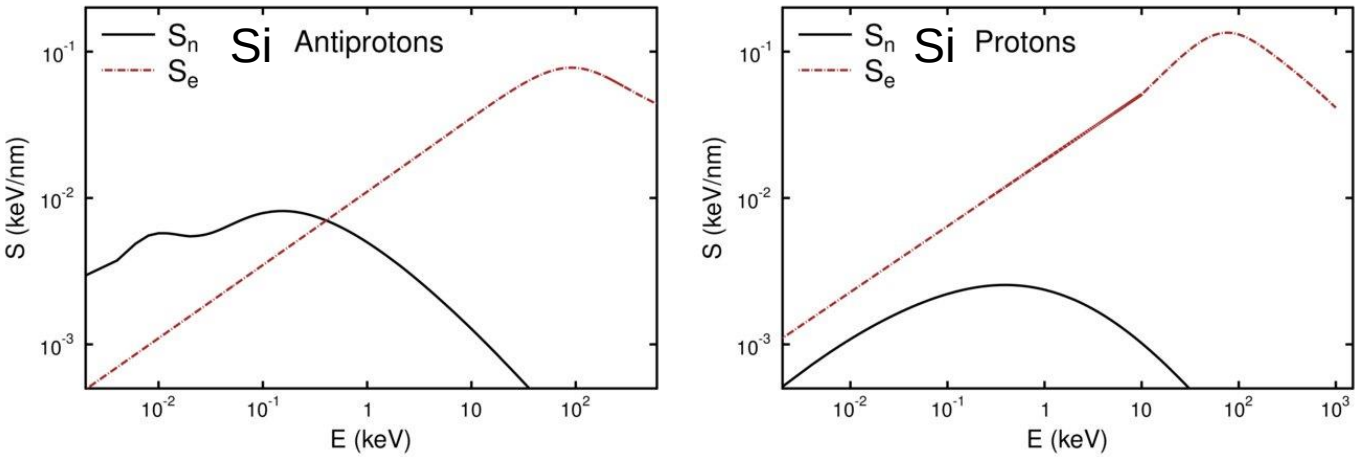
- Antiprotons present an interesting special case in nuclear stopping theory
- Because the charge of the antiproton is negative, they will be attracted to the regular atom nucleus
- Nordlund et al [Phys. Rev. A **96**, 042717 (2017)] showed that the even accounting for the screening by electrons, the antiproton-atom interparticle potential is attractive at all distances



- The binary collision integral cannot be used since the scattering is inwards (square root would become imaginary)

A special case: nuclear stopping power of antiprotons

- Using molecular dynamics iteration of the scattering process between antiprotons and atoms, it is possible to determine the energy transfer T and hence the nuclear stopping power
  - Contrary to the case of protons, for antiprotons the nuclear stopping power is stronger than the electronic stopping power at very low energies
    - Reason: stronger scattering energy transfer due to attractive potential and longer screening length



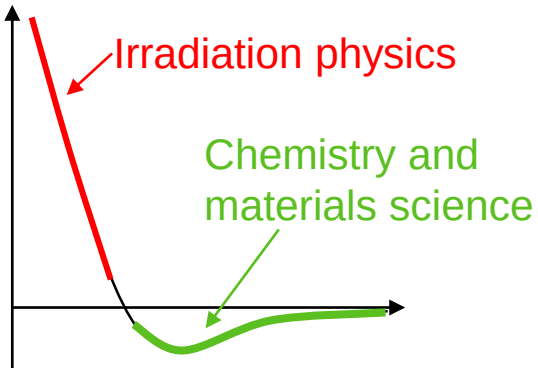
[Nordlund *et al*, Phys. Rev. A **96**, 042717 (2017)]

4.3 Role of interatomic potential

- The final solution shows that the actual scattering angle is determined from the interatomic potential:

$$\Theta = \pi - \int_{-\infty}^{+\infty} \frac{bdr}{r^2\sqrt{1-\frac{b^2}{r^2}-\frac{V(r)}{E_{CM}}}} = \pi - 2\int_{r_{\min}}^{+\infty} \frac{bdr}{r^2\sqrt{1-\frac{b^2}{r^2}-\frac{V(r)}{E_{CM}}}}$$

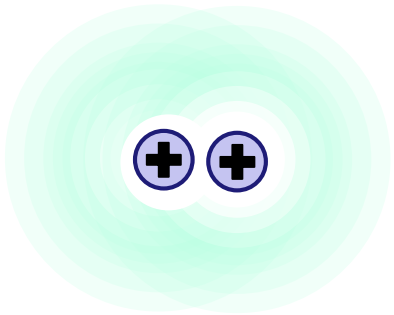
- Hence good knowledge of the interatomic potential $V(r)$ is crucial for being able to accurately calculate the stopping and energy transfer of atoms in solids
- For keV and MeV energies, the solution is fully dominated by the repulsive part of the potential



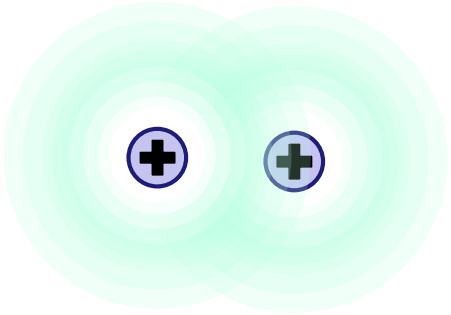
Repulsive potentials

- The origin of the repulsive potential can be understood by considering the structure of an atom: a positive nucleus of size ~ 1 fm surrounded by an electron cloud of size ~ 1 Å.
- Assume the shells are filled and the van der Waals interaction is negligible: then the interactions go as follows:

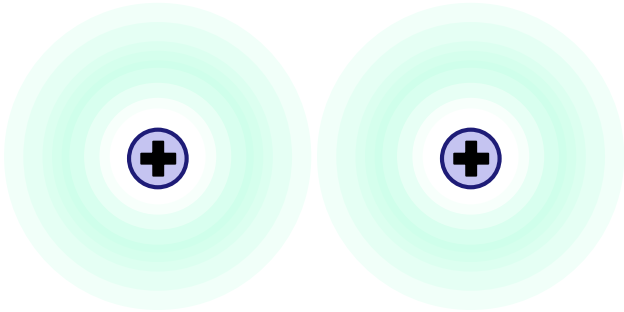
Atoms very close to each other => pure Coulomb repulsion



Intermediate distances => electron clouds partly screen the Coulomb repulsion



Atoms far from each other => complete screening, no interaction



Pure Coulomb potential – Rutherford scattering

- At the very smallest distances, the pure nuclei see each other and one can consider the problem with the ‘pure’ Coulomb potential

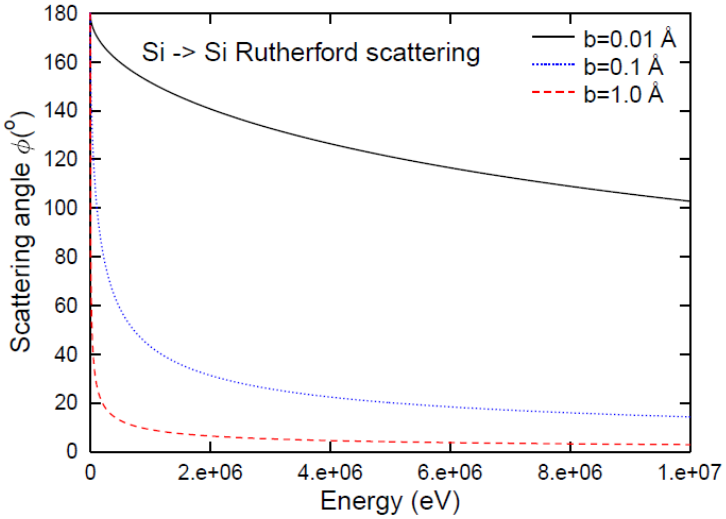
$$V(r) = \frac{1}{4\pi\epsilon_0}\frac{Z_1 Z_2 e^2}{r}$$

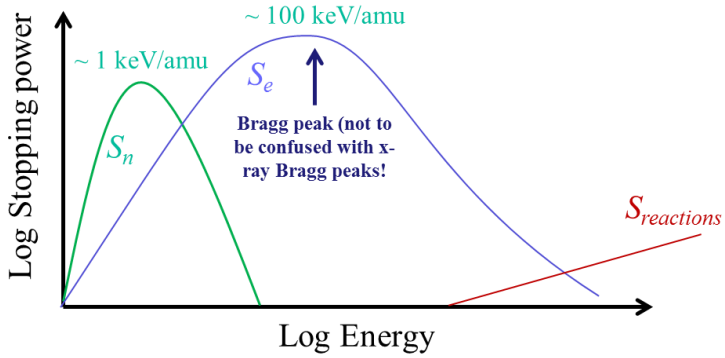
- In this case the scattering integral is actually solvable exactly analytically [Was page 34-36]. The solution for the scattering angle can be from the solution written as

$$\varphi = 2\arcsin\left(\sqrt{\frac{1}{1+\frac{4b^2 M_2 E_i}{Z_1 Z_2 e^2 (M_1+M_2)}}}\right)$$

Reason to decrease of nuclear stopping

- This shape has the feature that the scattering angle decreases with increasing energy (see adjacent figure)
- This explains why the nuclear stopping starts decreasing above some energy: the ion is deflected less and transfers relatively less energy => less energy deposition/stopping
- Qualitative explanation: “ion is faster => less time near another atom => less time to transfer energy”





Screened Coulomb potentials

- From the physical picture, it becomes natural to write the interaction for larger distances in the form of a **screened** (*avskärmad / varjostettu)* Coulomb potential

$$V(r) = \frac{1}{4\pi\epsilon_0}\frac{Z_1 Z_2 e^2}{r}\varphi(r/a)$$

- Here the screening function φ is a function that should become 1 when $r=0$ and 0 when $r=\infty$
  - This form fills the requirement that the potential becomes a pure Coulomb potential at short distances
- Here Z_1 and Z_2 are the charges of the interacting nuclei, and r the distance between them; a is the so-called screening parameter.

[These three pages are largely from the wikipedia page Stopping power (particle radiation) sections written by Kai Nordlund

Screened Coulomb potentials

- A large number of different repulsive potentials and screening functions have been proposed over the years, some determined semi-empirically, others from theoretical calculations.
- A very widely used repulsive potential is the one given by Ziegler, Biersack and Littmark, the so-called **ZBL repulsive potential**.
- It has been constructed by fitting a universal screening function to theoretically obtained potentials calculated for a large variety (~ 500) of atom pairs using so called Thomas-Fermi electron structure calculations from the 1970's.

The ZBL potential

- The ZBL screening parameter and function have the forms

$$a = a_u = \frac{0.8854 a_0}{Z_1^{0.23} + Z_2^{0.23}}$$

$$\varphi(x) = 0.1818 e^{-3.2x} + 0.5099 e^{-0.9423x} + 0.2802 e^{-0.4029x} + 0.02817 e^{-0.2016x}$$

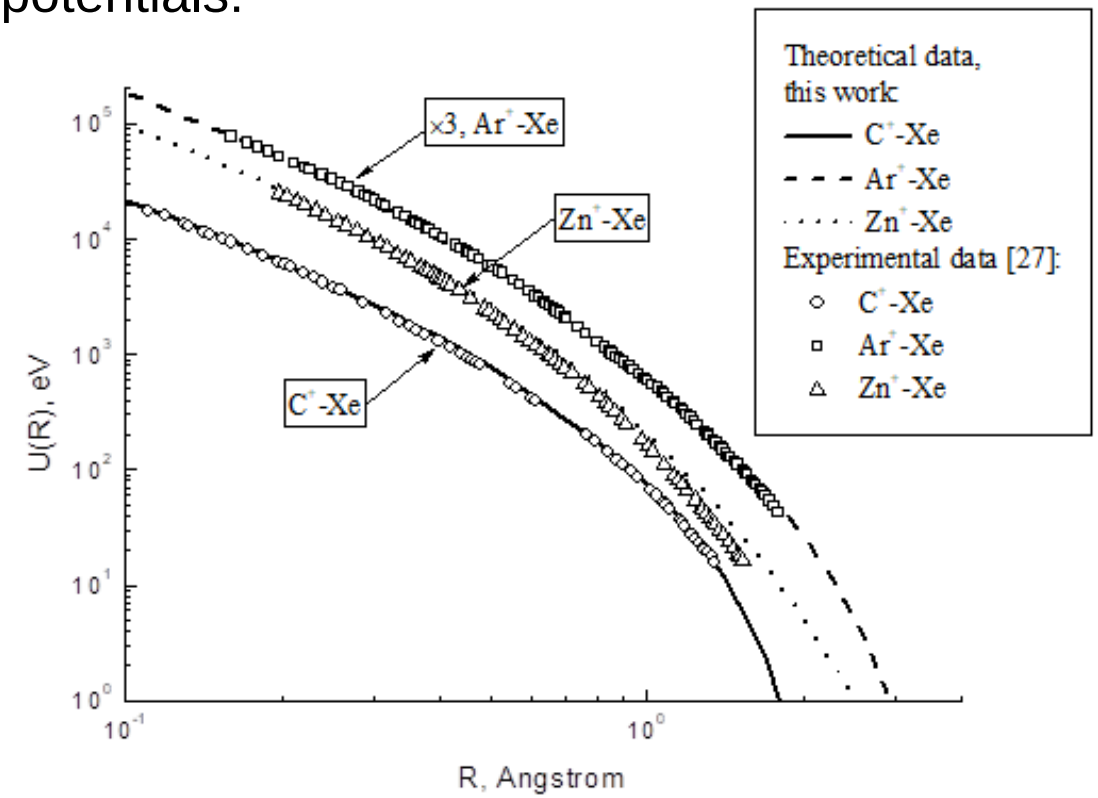
  where $x = r/a_u$, and a_0 is the Bohr atomic radius = 0.529 Å.

- The standard deviation of the fit of the universal ZBL repulsive potential to the theoretically calculated pair-specific potentials it is fit to is 18% above 2 eV [ZBL book]
- Even more accurate (~1%) repulsive potentials can be obtained from self-consistent total energy calculations using density-functional theory, but much of the time the ZBL potential is ‘good enough’

[K. Nordlund, N. Runeberg, and D. Sundholm, Nucl. Instr. Meth. Phys. Res. B 132, 45 (1997)].

Repulsive potentials from experiments?

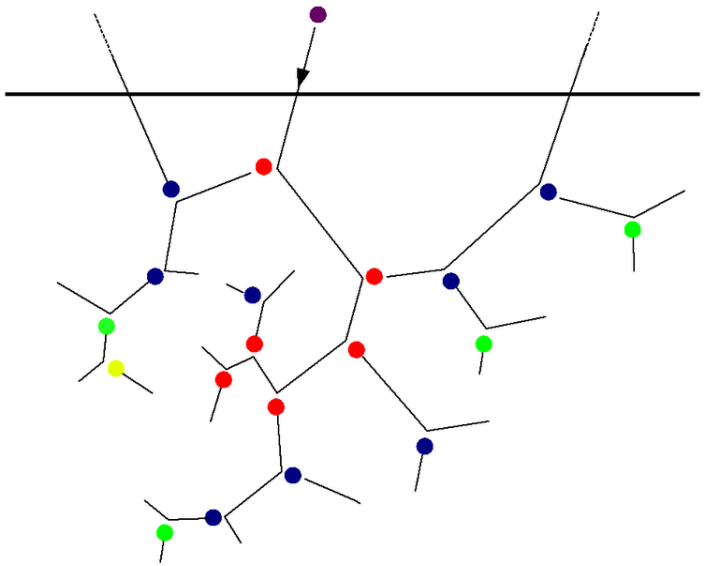
- It is also possible to determine the repulsive part of the interatomic potential from gas phase scattering experiments
- Recent example of experimental data compared to Dmol DFT repulsive potentials:



[A. N. Zinoviev and K. Nordlund, Nucl. Instr. Meth. Phys. Res. B 406 (2017) 511]

4.4. Binary collision codes like SRIM

- What Binary collision approximation (BCA) codes like SRIM do is follow the passage of an ion and its recoils, collision after collision in space
- The position and impact parameter of the next colliding atom is selected with a Monte Carlo approach selecting the next colliding atom according to the density of the material
- This gives a picture of the **collision cascade** (*kollisionskaskad / törmäyskaskadi*) formed by the set of atoms



Picture: wikipedia by Kai Nordlund]

Energy transfer

- The binary collision calculations gave (for any interatomic potential)

$$T = 4\frac{M_1 M_2}{(M_1 + M_2)^2} E_i \cos^2 \theta_2$$

where E_i is the initial energy of the particle of mass m, T is the energy transferred to the atom of mass M, and θ is the scattering angle in center-of-mass coordinates.

  - This equation was already given in section 2 for nuclei

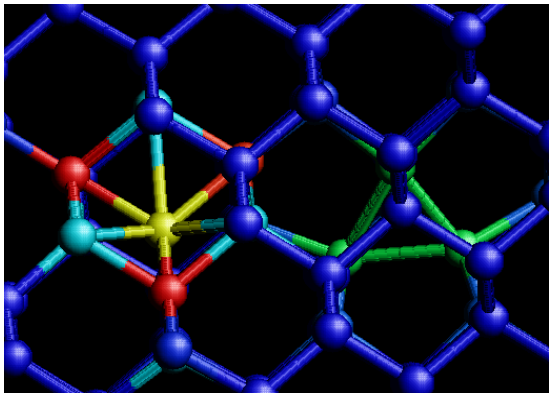
- The energy transfer T is what eventually may lead to damage production

Binary collision damage model

- In BCA codes like SRIM the model for damage production is simple: if the energy of a recoil exceeds a certain threshold value, known as the **threshold displacement energy (***förskjutningsgränsenergi / siirtymäkynnysenergia***)** or the displacement energy or the threshold energy, it assumes a **vacancy (***vakans/vakanssi***)** (empty lattice site) is produced where the recoil atom was initially
- The threshold displacement energy (TDE) can be measured experimentally using electron irradiation to find the threshold at which damage starts to be produced
- The TDE's are typically between 10 and 50 eV in elemental materials, and in BCA models assumed to be a constant for the material

4.5 The threshold displacement energy

- The threshold displacement energy is the smallest amount of kinetic energy needed to permanently displace an atom from its lattice site

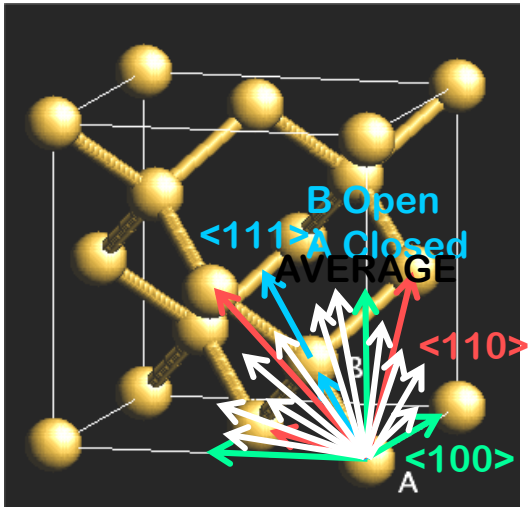


- The full concept is a 3D function:

$$p(T,\alpha,\varphi) = 0, \quad T < T_d(\alpha,\varphi)$$
$$= 1, \quad T \geq T_d(\alpha,\varphi)$$

$$T_{d,\text{ave}} = \text{ave}\left(T_d(\alpha,\varphi)\right)$$

$$T_{d,\text{min}} = \min\left(T_d(\alpha,\varphi)\right)$$



Different varieties of the threshold energy

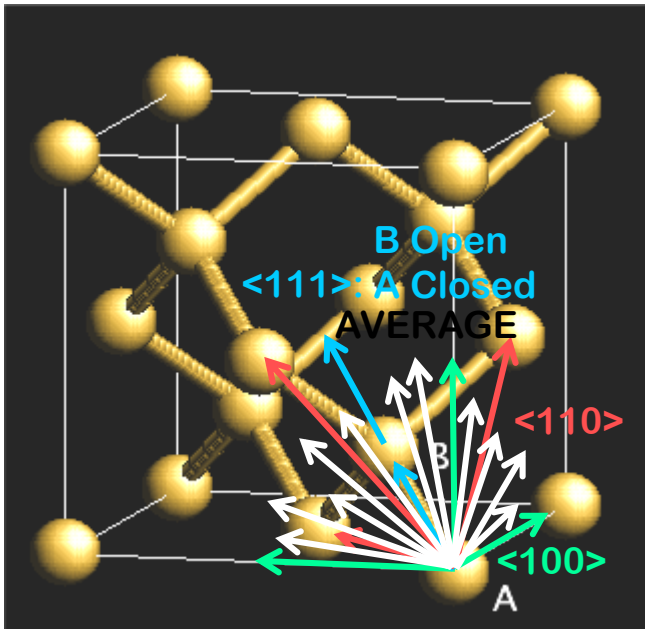
- One can in fact define several physically different threshold energies:
- Minimum vs. average threshold displacement energy:
  - Direction-specific thresholds: $T_{d,100}$, $T_{d,110}$, …
  - Average threshold displacement energy:

$$T_{d,\mathrm{ave}} = \mathrm{ave}\left(T_d(\alpha,\varphi)\right)$$

  - Minimum threshold displacement energy:

$$T_{d,\mathrm{min}} = \min\left(T_d(\alpha,\varphi)\right)$$

    - Usually in one of the principal lattice directions



[K. Nordlund, J. Wallenius, and L. Malerba, Nucl. Instr. Meth. Phys. Res. B 246, 322 (2005)]

Threshold displacement energy is not really a constant

- Due to thermal vibrations and crystal-direction specificity, the TDE is not even a monotonously rising function

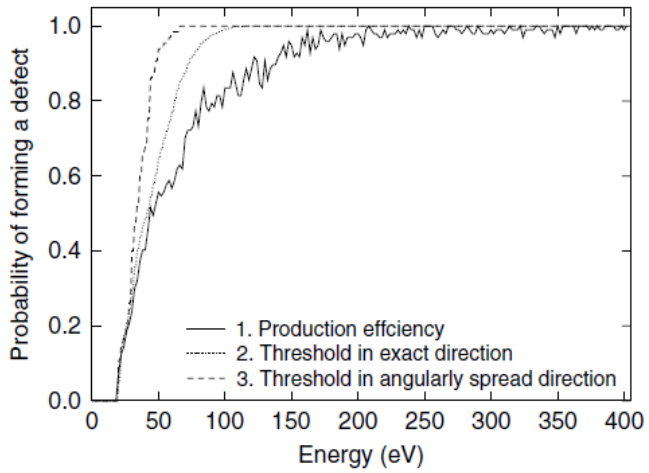


Fig. 2. Probability to form a defect at a given energy calculated in three different ways (see text) with the ABC potential.

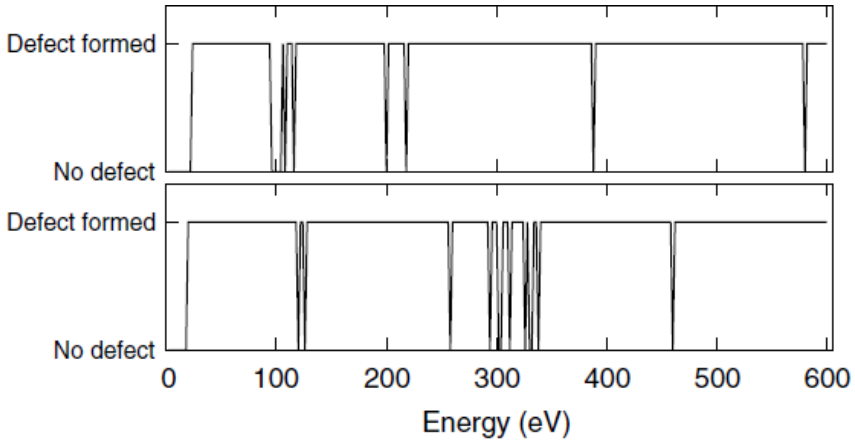
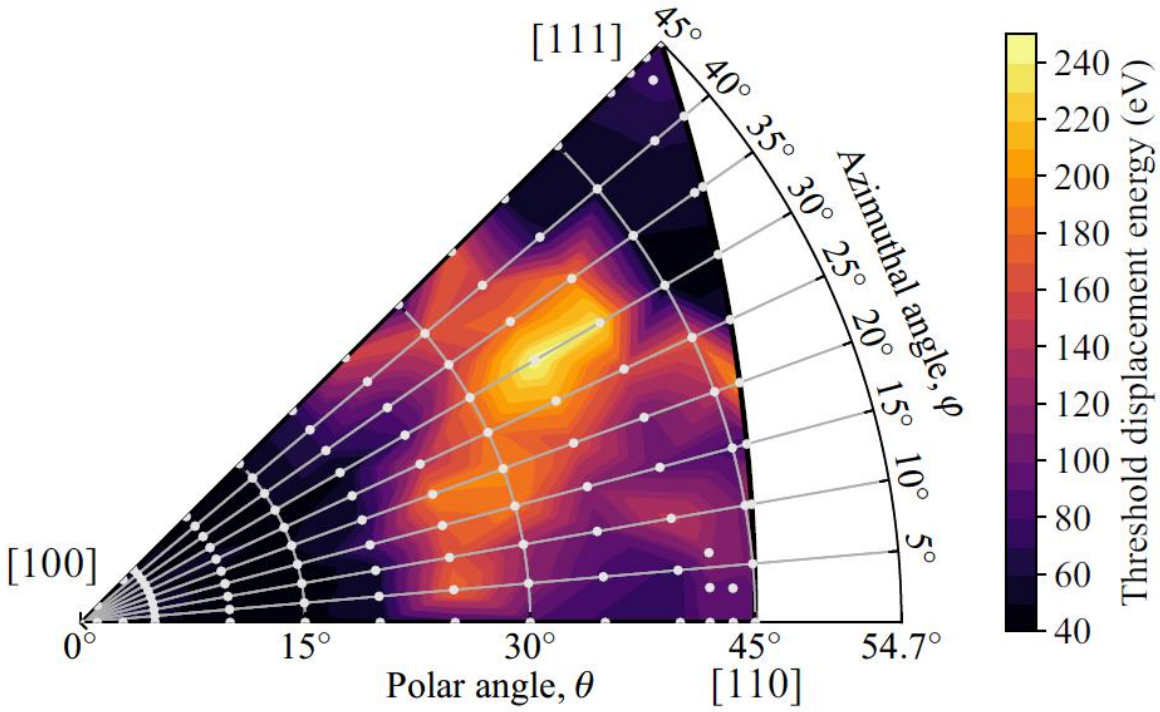


Fig. 1. Probability to form a defect for four recoils in Fe modelled with the ABC potential, as a function of recoil energy. Note that the data illustrates specifically the probability to form *at least* one defect; at the higher energies in many cases more than one defect is formed. In each of the four cases the initial state of the simulation is identical, including identical thermal atom displacements, except for the initial ion energy which is raised in steps of 2 eV.

[K. Nordlund, J. Wallenius, and L. Malerba, Nucl. Instr. Meth. Phys. Res. B 246, 322 (2005)]

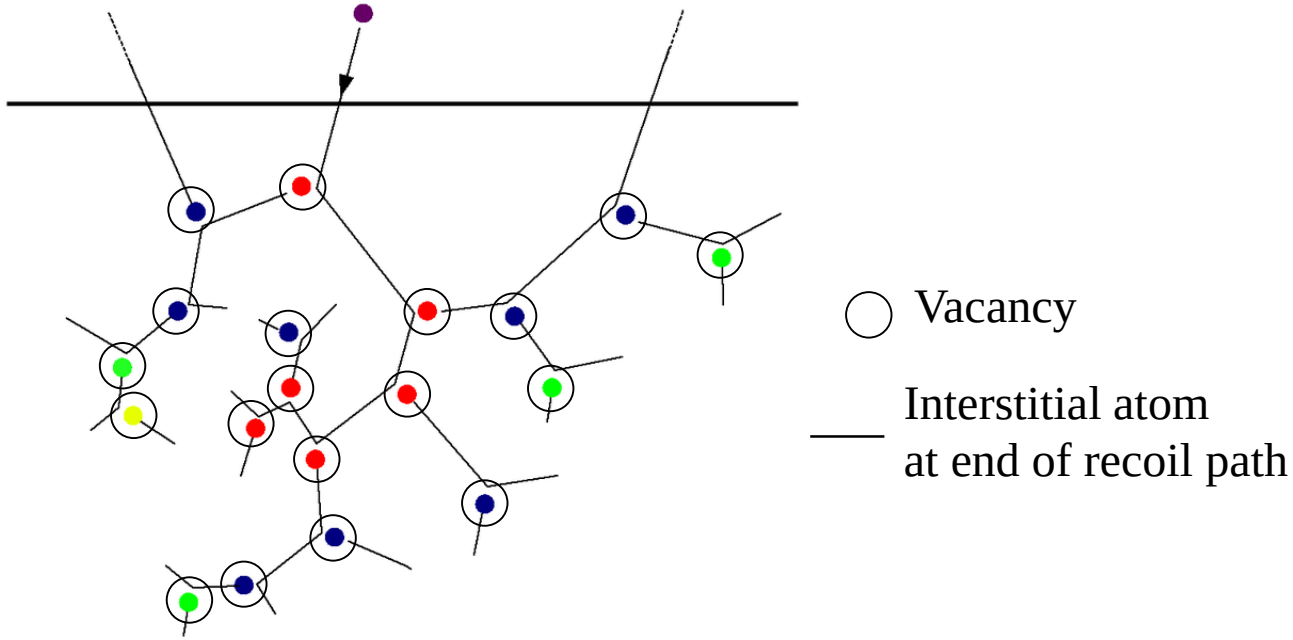
Example data: threshold displacement energy in W determined over all crystal directions



- (This map was calculated with a machine learned interatomic potential, which in 2019 was a state-of-the-art method. The results also agree with DFT calculations and experiments where available) [J. Byggmästar *et al*, Phys. Rev. B **100**, 144105 (2019)]

BCA model for damage production

- To repeat, the BCA model for damage production is that each recoiled atom above the threshold energy leaves behind a vacancy, and becomes itself either an **interstitial atom** (*interstitiell atom / välisija-atomi*) or is sputtered
  - The combination vacancy+interstitial is called a **Frenkel pair**



4.6. The Kinchin-Pease and NRT equations for damage production

- The BCA model for damage production assumes independent collisions, which means it natural to think that the actual damage production is linearly proportional to energy above the threshold
- This leads to the **Kinchin-Pease model** for damage production for a nuclear damage energy of T

$$N(T) = \begin{cases} 0 & \text{when} \quad T < E_d \\ 1 & \text{when} \quad E_d < T < 2E_d \\ \dfrac{T}{2E_d} & \text{when} \quad 2E_d < T < \infty \end{cases}$$

where E_d is the threshold displacement energy.

[Kinchin and Pease, Rep. Prog. Phys. 18 (1955) 1]

The Kinchin-Pease and NRT equations for damage production

- The K-P model was later modified by Norgens, Robinson and Torrens based on BCA simulations of the probability of a new recoil filling in a vacancy to the slightly modified so called NRT form to read:

$$N_{NRT}(T) = \begin{bmatrix} 0 & \text{when} & T < E_d \\ 1 & \text{when} & E_d < T < 2E_d \\ \dfrac{0.8\,T}{2E_d} & \text{when} & 2E_d < T < \infty \end{bmatrix}$$

- The NRT model includes using the Lindhard energy partitioning, i.e. $T = f(E_{PKA})$ where $f(\quad)$ is the function telling which fraction of the PKA energy E_{PKA} is lost to electronic stopping
- There is even a standard behind this form

Designation: E 693 – 01 (Reapproved 2007)

Standard Practice for
Characterizing Neutron Exposures in Iron and Low Alloy Steels in Terms of Displacements Per Atom (DPA), E 706(ID)[1]

The dpa concept

- Damage is very commonly given in the form of **displacements-per-atom (dpa)** (*förskjutningar-per-atom, siirtymiä atomia kohden*)
- The standard way to calculate this is to calculate the total nuclear damage energy deposition T (i.e. excluding electronic energy loss) in a given volume, then use the NRT-dpa equation to calculate the number of defects (”displacements”) in this volume. This number divided by the number of atoms in the same value defines the dpa value

The arc-dpa form

- However, during the last ~30 years it has become clear that the NRT form for calculating dpa's is badly off in metals!
  - This is due to recombination, which we will return to in detail in section 5
- This led an OECD Nuclear Energy Agency working group to devise a "athermal-recombination corrected dpa", arc-dpa equation of the form

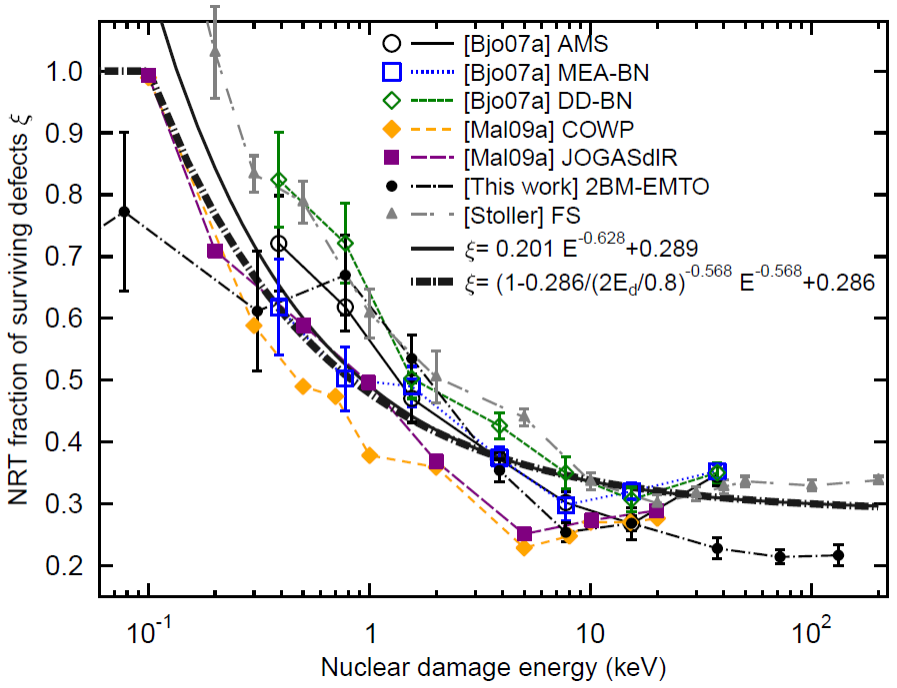
$$N_{d,arcdpa}(T) = \begin{bmatrix} 0 & \text{when} & T < E_d \\ 1 & \text{when} & E_d < T < 2E_d \\ \frac{0.8\,T}{2E_d}\xi(T) & \text{when} & 2E_d < T < \infty \end{bmatrix}$$

$$\xi(T) = \frac{1 - c_{arcdpa}}{(2E_d/0.8)^{b_{arcdpa}}} T^{b_{arcdpa}} + c_{arcdpa}$$

[Nordlund, Zinkle, et al. Nature communications **9**, 1084 (2018)]

Arc-dpa fit to damage production data

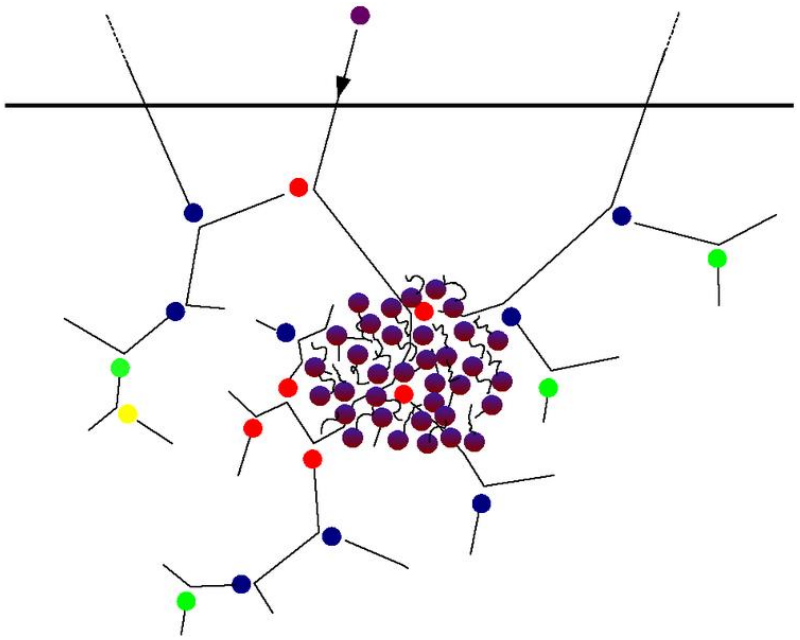
- This modified form fits damage production results in metals much better than the original NRT-dpa equation
  - In the plot below, the thick line is the new result fit to the data points, while the NRT-dpa equation would give 1 for all energy values



[Nordlund et al, J. Nucl. Mater. **512**, 450 (2018)].

Limitations of the BCA model of damage prediction

- Due to its nature of modelling only binary collisions, the BCA approximation breaks down when the ion and recoil energies become so low that atoms collide with many atoms simultaneously (many-body collisions)
- For the same reason, it cannot tell anything about the precise atomic structure of defects
- How to obtain such information will be described in the next section



Problems in SRIM damage models

- **Major caveat:** the SRIM software has internal inconsistencies between its own damage models
  - Roger Stoller *et al* [Nucl. Instr. Meth. Phys. Res. B 310 (2013) 75] showed that the ”number of vacancies” given by SRIM for the exact same irradiation condition can vary by a factor of 2 depending on whether the code is run in full cascade or ”Quick Kinchin-Pease” mode
    - This paper did not explain the reason
  - In 2019 William J. Weber and Yanwen Zhang [Current Opinion in Solid State & Materials Science 23 (2019) 100757] showed that the reasons are that the ”quick damage mode” uses the Lindhard model for energy partitioning, which is based on a different electronic and nuclear stopping models than those used in the ”full cascade” mode, and that the modified Kinchin-Pease model used to calculated number of displacements from the damage energy is based on an inherent assumption that there is a binding energy equal to the threshold displacement energy.
    - W. J. Weber also showed in the same work that two open source full cascade BCA codes (iradina and IM3D) give consistent results with the SRIM full cascade mode: that mode works reasonably

Problems in SRIM damage models

- To be fair to SRIM, the SRIM book does state that the ”K-P Quick calculation should only be used “if you do not care about details of target damage” “
- It is especially important to note that the K-P model and Lindhard partitioning are not even meant to be valid for multi-elemental targets => they should not be used for alloys and compounds at all
- Conclusion: for SRIM damage calculations, either use the full cascade mode, or do not use SRIM for damage calculations at all
  - They anyway are not physically realistic, real damage is always more complicated (this will be apparent in next sections of this course)
  - The energy deposition calculations are, however, quite reliable, and can be used as a basis for a dpa or arc-dpa calculation
- If one does use SRIM, one should always describe very precisely how it was done (SRIM version, calculation mode), otherwise the results are not reproducible

What should you have learned from this section?

- Understand the picture of binary collisions in solids
- Know how the binary collision equations are solved for the scattering angle
- Know the basics of repulsive interatomic potentials
- Know how a binary collision model treats damage production
- You know the concept of threshold displacement energies and analytical damage models based on these
- You know what the dpa concept is
- You know that SRIM has inconsistencies in its damage models, and in particular that the Kinchin-Pease model should not be used for alloys at all