HIP

Multiscale atomistic simulations of radiation effects in materials

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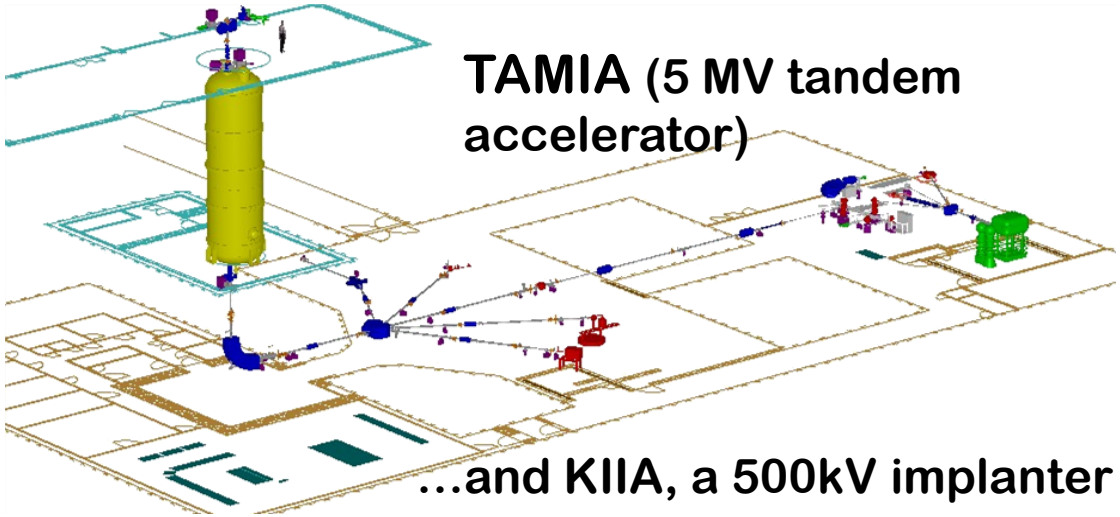
UNIVERSITY OF HELSINKI
KUMPULA CAMPUS
Accelerator laboratory

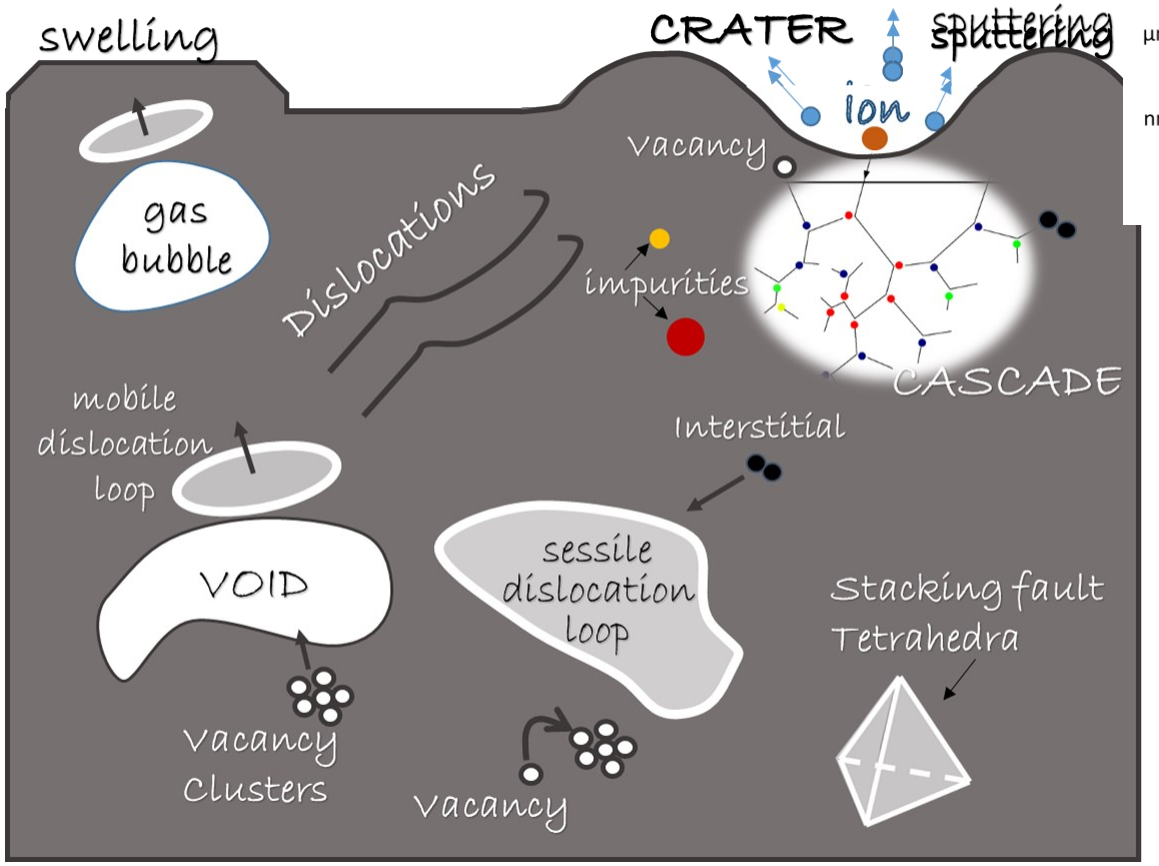
Accelerator Laboratory of the University of Helsinki

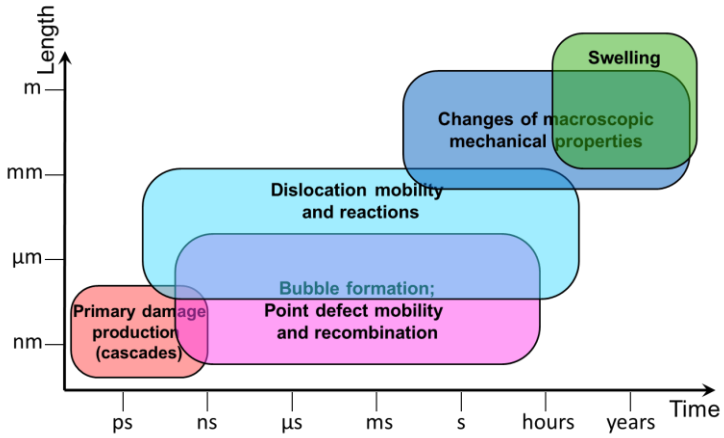
- Accelerators: 5 MeV tandem, 500 kV implanter
- Other equipment: AFM, sputter deposition, cluster ion source
- Positron accelerator
- Magnetron sputtering equipment
- About 60 scientists
- Main areas:
  - Materials physics
  - Nanoscience



https://www2.helsinki.fi/en/researchgroups/helsinki-accelerator-laboratory

Multiscale changes in materials under irradiation

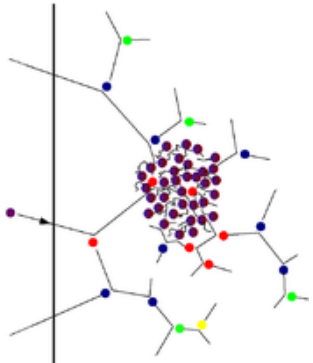


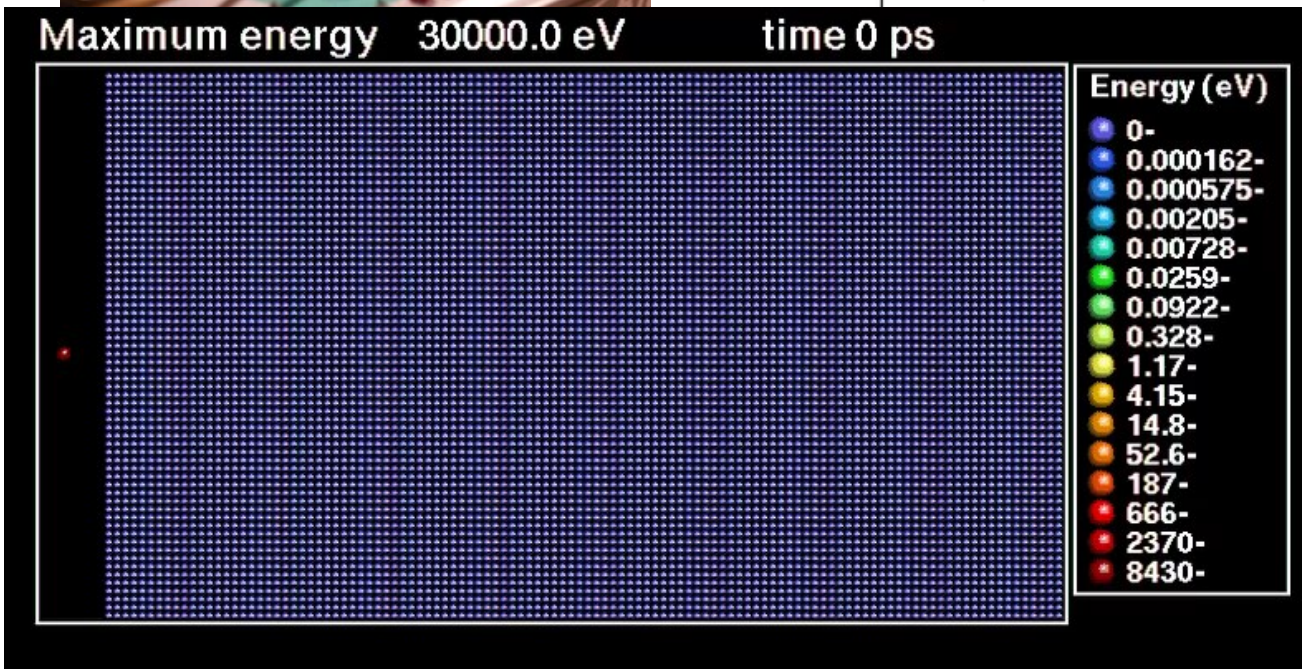


To model radiation effects on atomic level…

- One needs to be able to handle:
  1) keV-energy collisions between nuclei
  2) Energy loss to electronic excitations
  3) Transition to high-pressure and high-T thermodynamics (E_{kin} ~ 1 eV)
  4) Realistic equilibrium interaction models
  5) Phase changes, segregation, sputtering, defect production…
  6) Long-term relaxation of defects
- Sounds daunting, but:
  - Steps 1 – 2 can be handled in a binary collision approximation simulation
  - Steps 1 – 5 can all be handled in the same molecular dynamics simulation
  - Step 6 requires kinetic Monte Carlo or rate theory

Atomic cascades in the core of the radiation damage physics





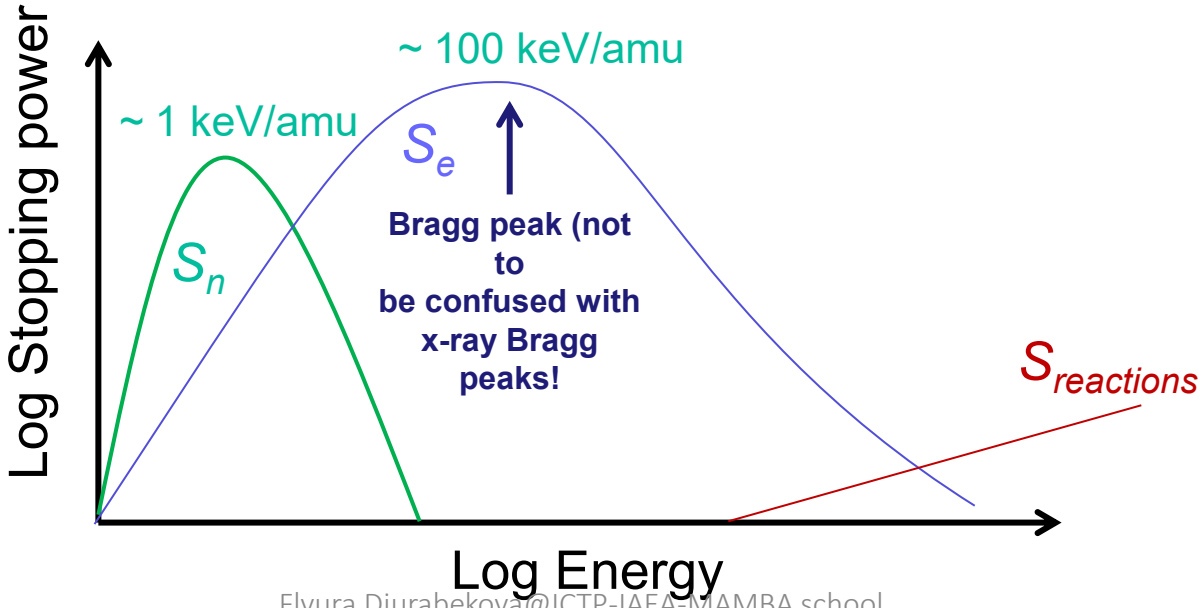
Example: 30 keV Xe ion damage in Au, 2D cross sectional view

Slowdown mechanisms for energetic particles in matter

- The process of ion slowdown in a material is considered in terms of "stopping power" (note the units of force, not of power ☺)

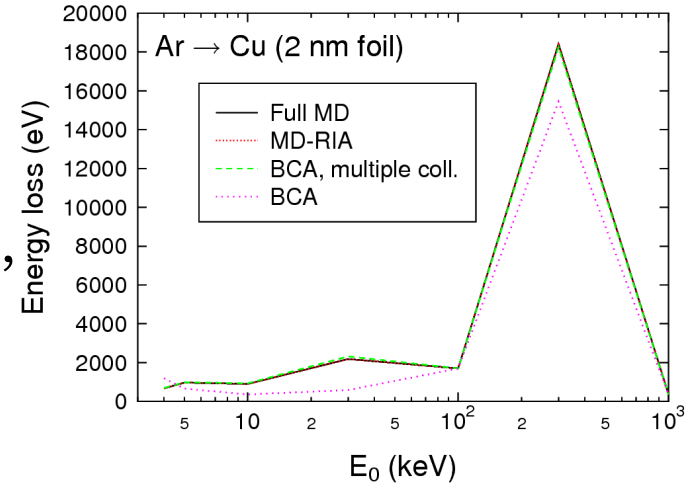
$$S = -\frac{dE}{dx} = S_n + S_e + S_{reactions}$$

S_n and S_e are fractions of energy spent on interaction with nuclei and the electrons



Energy losses

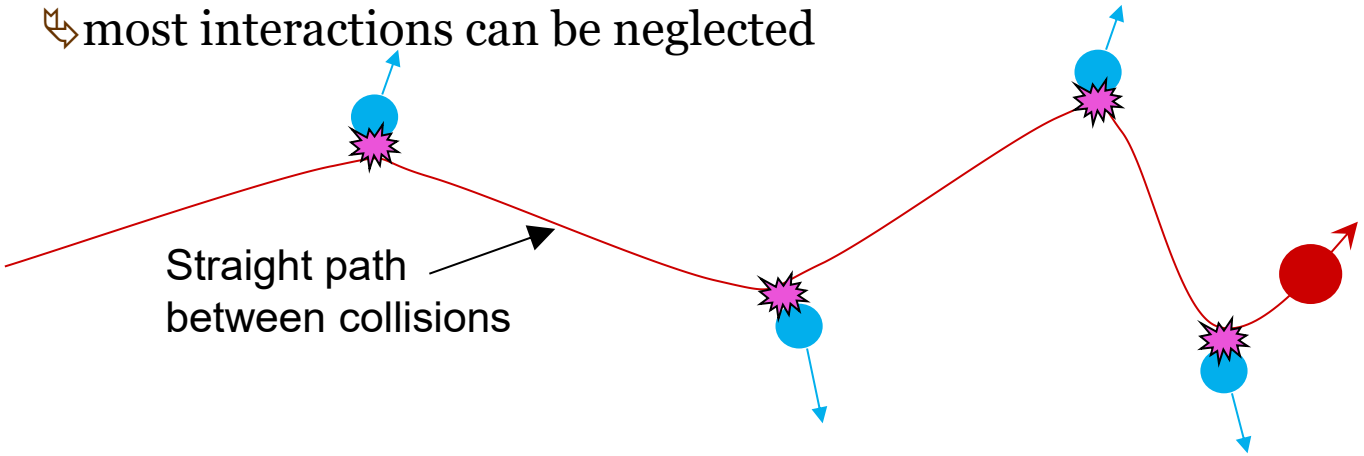
- The nuclear stopping power $S_n(E)$ is simply the average energy loss per unit path length travelled from all the collisions
  - In principle, it is always from all the multiple simultaneous collisions
- But for high ion/recoil energies ≫ 1 keV, the collision cross section becomes low, and a few binary collisions dominate the energy loss
- For the example case of Ar ->Cu, for $E \geq 100$ keV, single binary collision model very accurate



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

BCA = Binary collision approximation

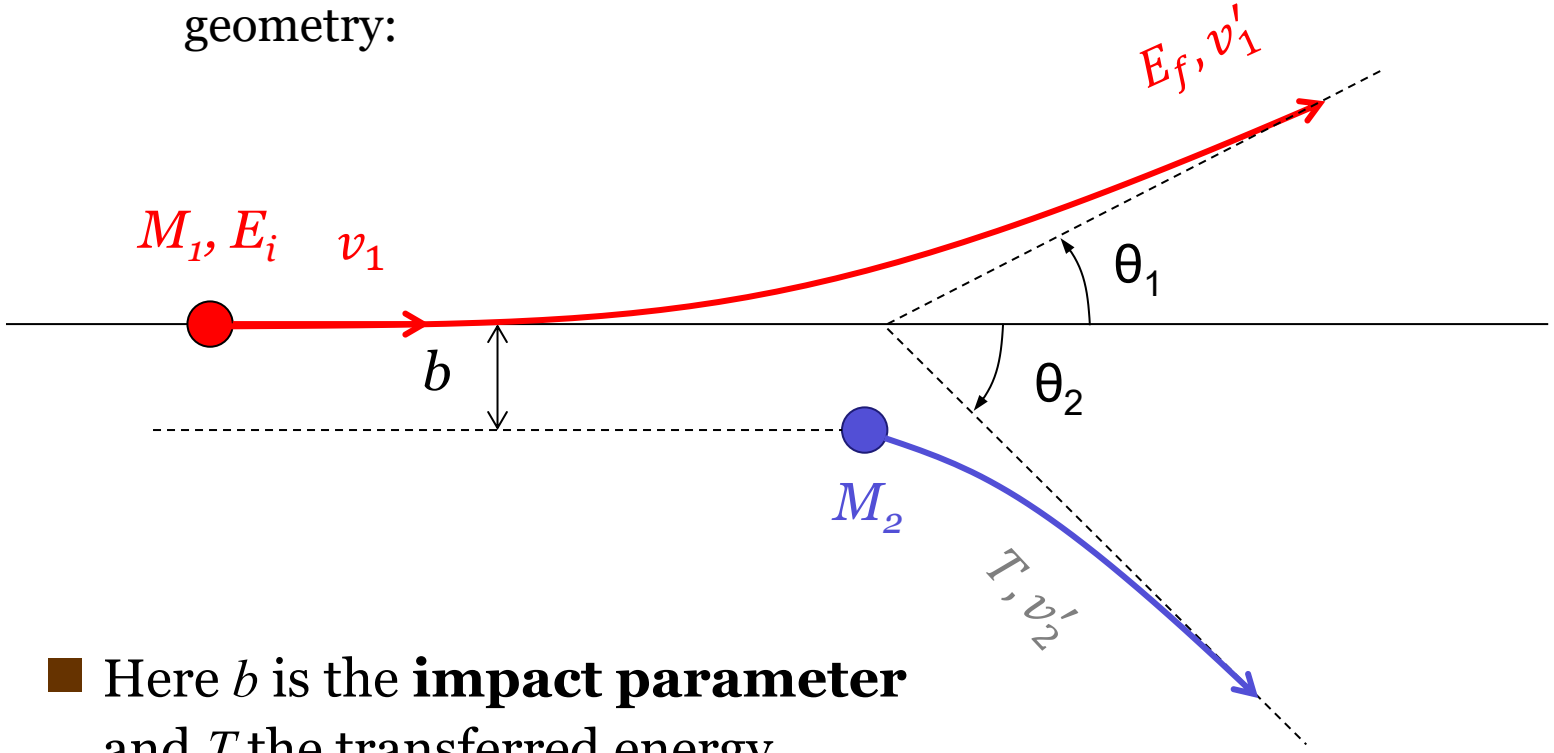
- BCA is the original way to simulate ion irradiation effects on a computer
  - Developed by Mark Robinson, ~1958
- In BCA, the collisions of an incoming ion are treated as a sequence of independent collisions ⇒ the ion motion is found by solving the classical scattering integral
- Based on the physics insight that at high energies, ion collision cross section with lattice atoms is low => it moves along straight path much of the time
  - most interactions can be neglected



[wikipedia page by K.Nordlund]

Basics of BCA

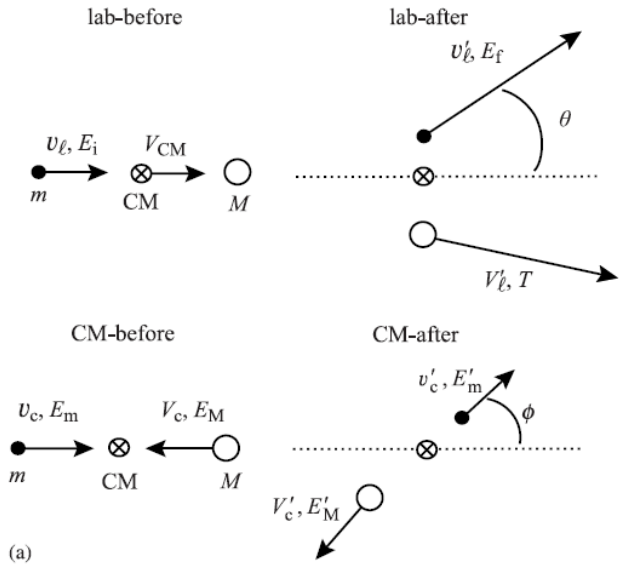
- The basic premise of BCA is following:
  - a moving atom with velocity v_1 of mass M_1 and initial energy E_i is impacting on an atom at rest of mass M_2 in the following geometry:



- Here b is the **impact parameter** and T the transferred energy

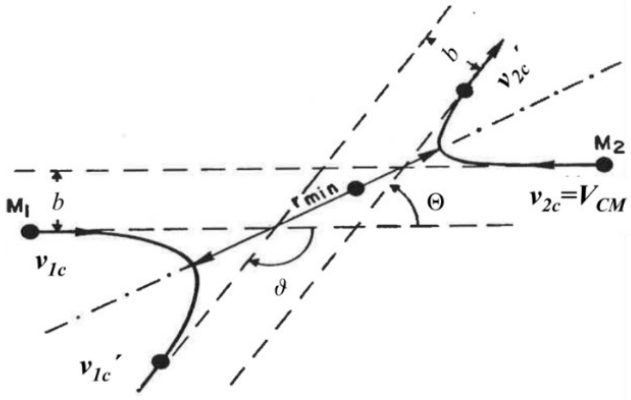
Basics of BCA

- The classical two-body scattering event is treated in the center-of-mass coordinates, solving the scattering integral in the full range of distances between the colliding atoms with the repulsive interatomic potential *V(r)*.
- Later on, the angle Θ is recalculated into the scattering angles for impacting atom and the tom in rest θ_1 and θ_2



Interatomic potential

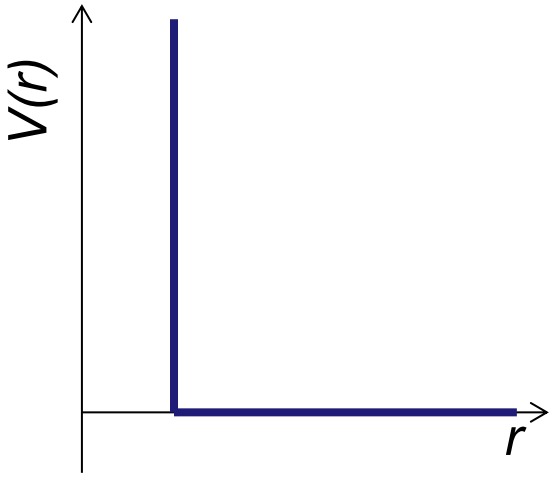
$$\Theta = \pi - \int_{-\infty}^{+\infty} \frac{bdr}{r^2\sqrt{1-\frac{b^2}{r^2}-\frac{V(r)}{E_{CM}}}} = \pi - 2\int_{r_{min}}^{+\infty} \frac{bdr}{r^2\sqrt{1-\frac{b^2}{r^2}-\frac{V(r)}{E_{CM}}}}$$



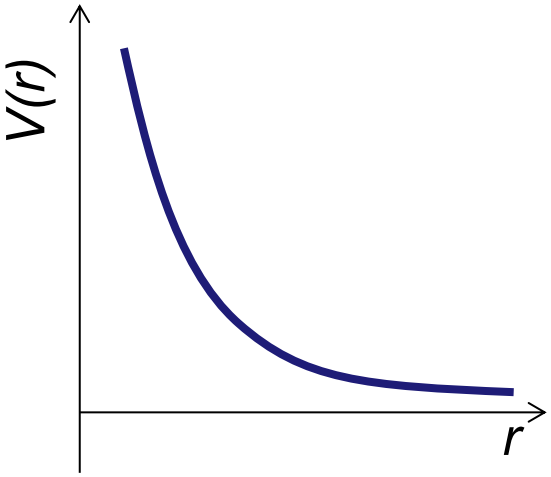
Central-force scattering

- 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:

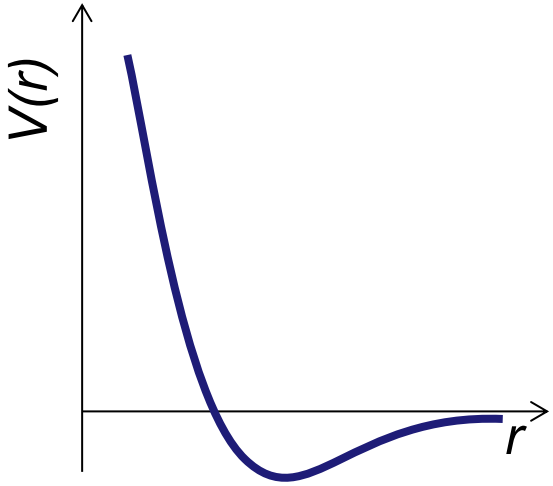
Hard-sphere potential



Purely repulsive potential



Potential with attractive well



Repulsive interatomic potential: Ziegler-Biersack-Littmark (ZBL)

- The ZBL screening parameter and function have the form

$$V(r) = \frac{1}{4\pi\varepsilon_0}\frac{Z_1 Z_2 e^2}{r}\varphi\left(\frac{r}{a}\right)$$

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

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

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

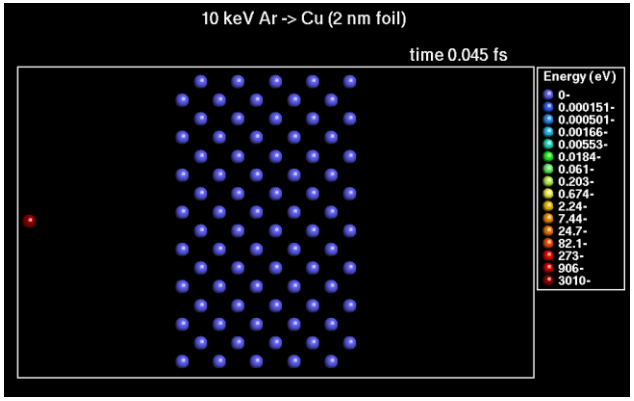
- The standard deviation of the fit of the universal ZBL repulsive potential to the theoretically calculated pair-specific potentials to which ZBL is fit is 18% above 2 eV[1]
- A more accurate (~1%) repulsive potentials can be obtained from self-consistent total energy calculations using density-functional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

[1]ZBL book

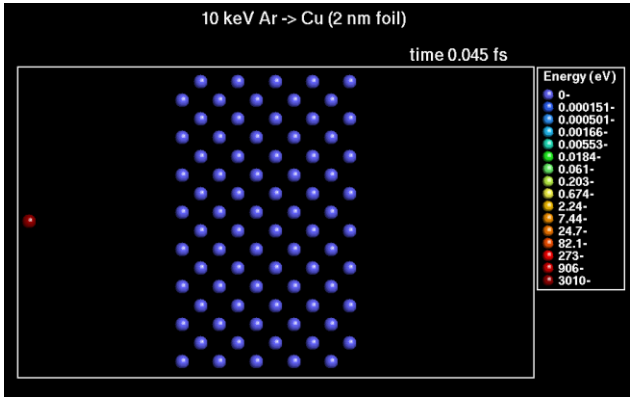
[2]K. Nordlund, N. Runeberg, and D. Sundholm, Nucl. Instr. Meth. Phys. Res. B 132, 45 (1997)

Comparison of binary vs multibody collisions

MD

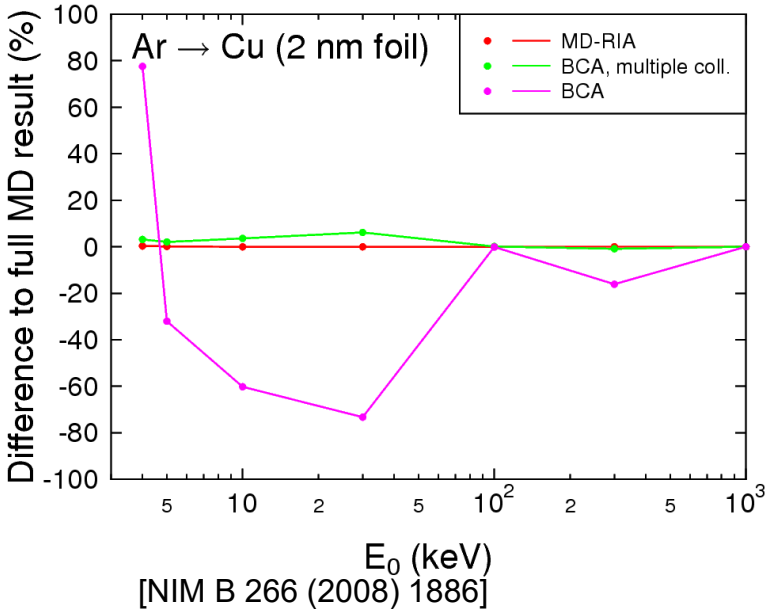


BCA-like



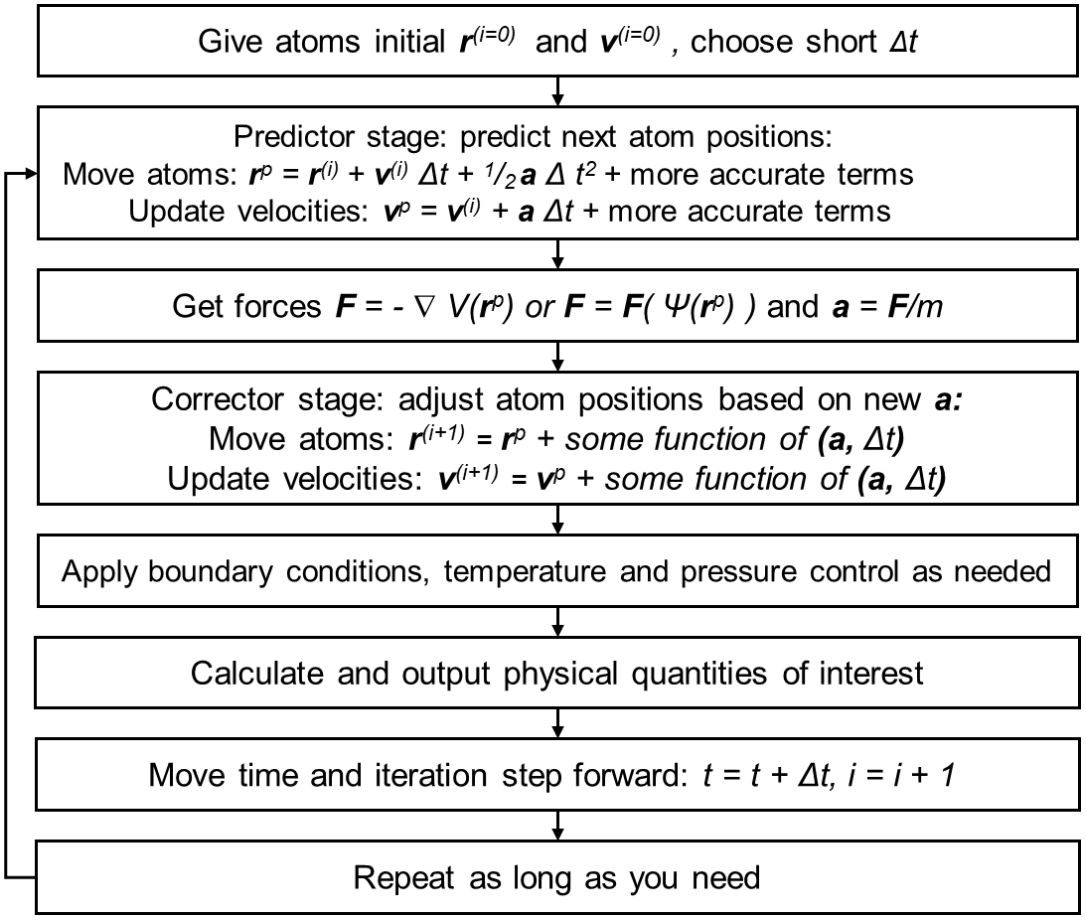
Example: 10 keV Ar -> Cu

- In the low energy range (5 – 10 keV Ar -> Cu) the difference can be very strong!
  - Energy losses are different even at 500 keV
  - Lower-energy recoils obviously missing from BCA



[NIM B 266 (2008) 1886]

Molecular Dynamics algorithm



- In Molecular Dynamics, we solve iteratively the Newton's equations for all atoms in the system.

Adative time step for simulation of radiation effects

- During ion irradiation simulations an energetic particle with the energy of several keV may cover distance of several Å, which is much greater than a single interatomic distance
- This will introduce significant temperature drift in the system
  - Pretty good rule of thumb: the fastest-moving atom in a system should not move further than 1/20 of the smallest interatomic distance per time step – typically about 0.1 Å
- Hence, it is strongly recommended to apply an adaptive timestep algorithm
- $\Delta t = \min\left(\frac{k_t}{v_{max}}, \frac{E_t}{F_{max} v_{max}}, 1.1\Delta t_{prev}, \Delta t_{eq}\right)$
- k_t = a specified maximally allowed distance on which an atom can move during a single step
- E_t = a maximal energy change in the system. Both parameters are set based on test simulations for energy conservation and are typically 0.1 Å and 30 eV, respectively.

[K. Nordlund, Comput. Mater. Sci. 3, 448 (1995)].

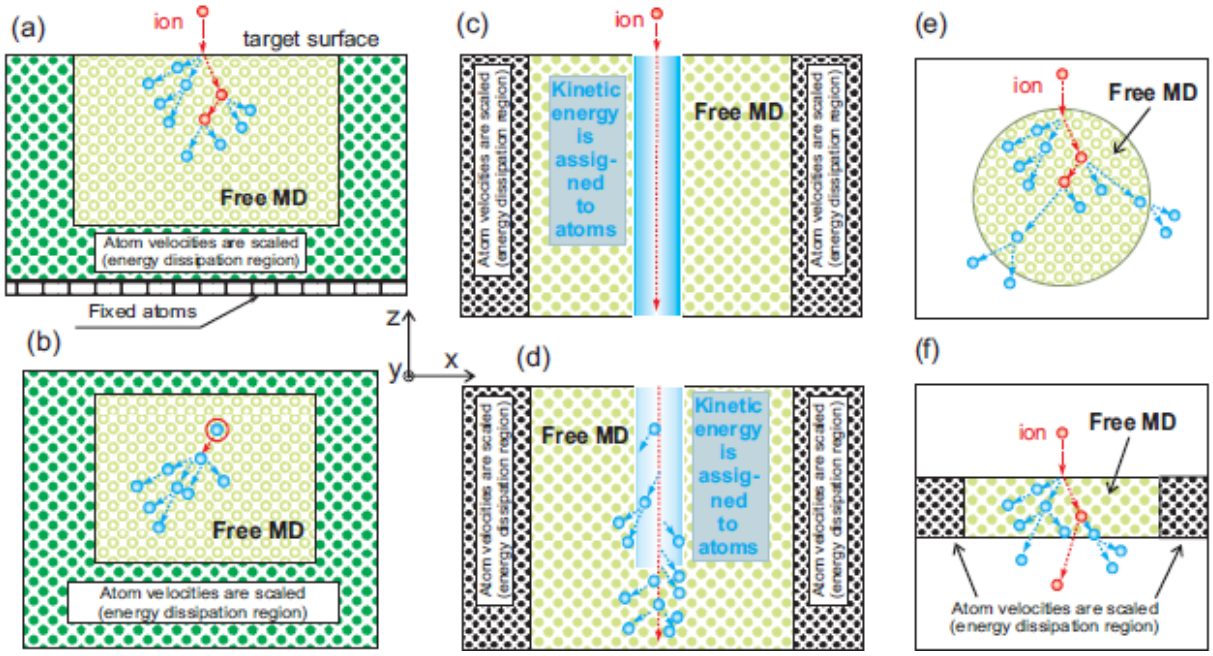
MD – Temperature and pressure control

- Controlling temperature and pressure is often a crucial part of MD
- "Plain MD" without any T or P control is same as simulating **NVE** thermodynamic ensemble
  - **In irradiation simulations NVE is the only correct approach to deal with the collisional phase !!**
- **NVT** ensemble simulation: temperature is controlled in a fixed volume
- **NPT** ensemble simulation: both temperature and pressure are controlled
  - Many algorithms exist: Andersen, Nosé-Hoover, Berendsen
  - Berendsen is very simple yet often good enough
  - Currently Nosé-Hoover is often preferred

MD irradiation temperature control

- Central part has to be in NVE ensemble, but on the other hand extra energy/pressure wave introduced by the ion or recoil needs to be dissipated somehow
- Exact approach to take depends on physical question:

a) surface, b) bulk recoil, c-d) swift heavy ion, e) nanocluster, f) nanowire



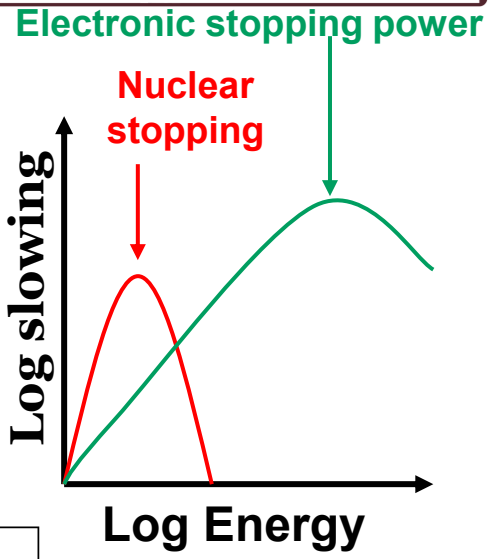
[A. V. Krasheninnikov et al., J. Appl. Phys. (Applied Physics Reviews) **107**, 071301 (2010).

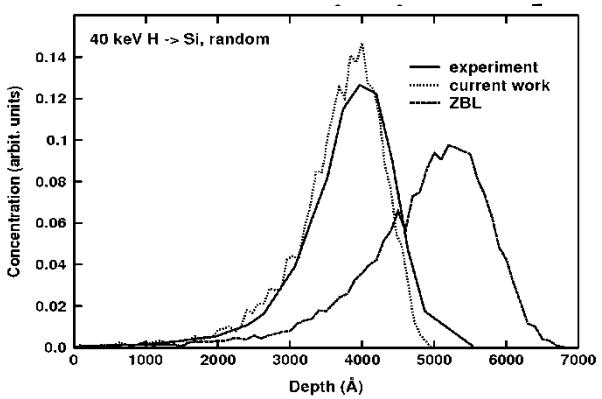
Energy loss to electronic excitations

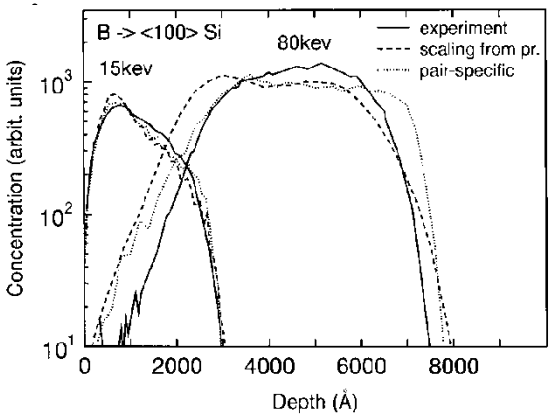
- The energy loss to electronic excitations = electronic stopping S can be included as a frictional force in MD simply as:

$$v^{(i+1)} = v^{(i)} - S(v)/m\Delta t$$

- It can also be compared directly to experiments via BCA or MD range or ion





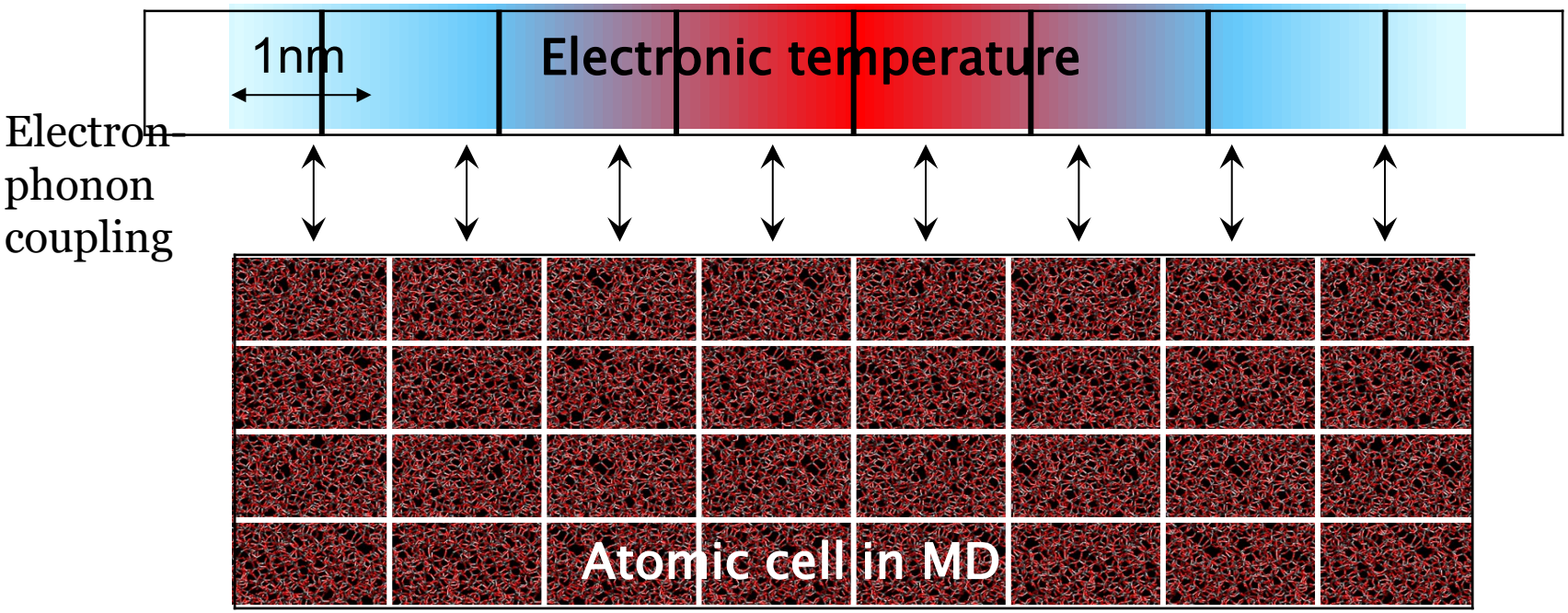


[J. Sillanpää, K. Nordlund, and J. Keinonen, Phys. Rev. B 62, 3109 (2000); J. Sillanpää J. Peltola, K. Nordlund, J. Keinonen, and M. J. Puska, Phys. Rev. B 63, 134113 (2000); J. Peltola, K. Nordlund, and J. Keinonen, Nucl. Instr. Meth. Phys. Res. B 217, 25 (2003); J. Peltola, K. Nordlund, and J. Keinonen, Nucl. Instr. Meth. Phys. Res. B 212, 118 (2003)]

Electronic losses within the MD algorithm

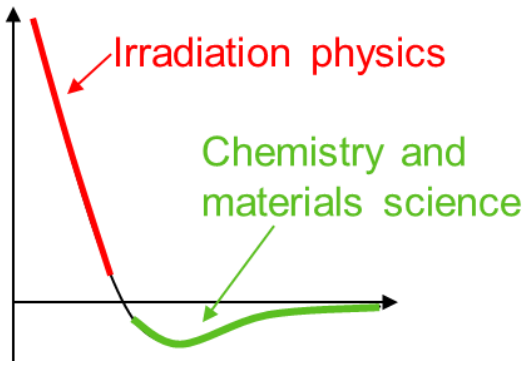
$$m_i \frac{\partial v_i}{\partial t} = F_i(t) + \xi m_i v_i; \qquad \xi = \frac{\frac{1}{n}\sum_{k=1}^{n} V_n G(T_e) \cdot (T_e^k - T_i)}{\sum_i m_i v_i^2}$$

As in [S. Ivanov and V. Zhigilei PRB **68** (2003) 064114], or via the Langevin thermostat as in [D. M. Duffy and A. M. Rutherford J. Phys: Condens. Matt. **19** (2007)]



Interatomic potentials to describe keV and MeV-energy collisions between nuclei

- To simulate the radiation effects, the potential must describe the physics/ chemistry of near-equilibrium and at very short distances.
- To handle the high-E collisions, one needs to know the high-energy repulsive part of the interatomic potential
  - For instance, the DFT methods can be used to calculate it within ~1% accuracy for all energies above 10 eV
  - So called "Universal ZBL" potential accurate to ~5% and very easy to implement
  - Fit directly within GAP potential
- Simulating this gives the ***nuclear stopping*** explicitly!



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

Classical formalism for equilibrium potentials suitable for different materials

- To describe chemical interactions (different nature of bonds etc.), the simple 2-body potentials are used only for noble gases
- Dominant are 3-body potentials, and increasingly 4-body are used
- Two major classes of potentials:
  - Tersoff-like: $V_i = \sum_{\text{neighbours}}[V_{\text{repulsive}}(r_{ij}) + b_{ijk}(r_{ij}, r_{ik}, \theta_{ijk})V_{\text{atractive}}(r_{ij})]$,

    where $b_{ijk} \propto \frac{1}{\sqrt{\text{coordination of } i}}$
  - Embedded-atom method-like (EAM): $V_i = \sum_{\text{neighbours}}[V_{\text{repulsive}}(r_{ij}) + F_i(\sum_j \rho(r_{ij}))]$
- Both can be motivated in the second momentum approximation of tight binding ("extended Hückel approximation" for chemistry applications)
  - Related to Pauling's theory of chemical binding

[K. Albe, K. Nordlund, and R. S. Averback, Phys. Rev. B 65, 195124 (2002)]

GAP machine-learning potentials

- Recently a compromise between the accurate, but computationally expensive, calculations using the DFT-MD methods and the less accurate, but computationally much more efficient methods have been found.
- Machine-learning Gaussian approximation potentials (GAP, see [A. P. Bartók & G. Csányi et al. 2010, 2013]) have been proven to be an improved alternative to the classical potentials
- Main ingredients for a ML potential:
  - A machine learning architecture
  - A way to quantify local atomic environment (descriptor)
  - Consistent set of training data (typically from DFT)

GAPs for pure BCC metals: W, Mo, Nb, Ta, V

Refit … like p … criptor … ic positions,

PHYSICAL REVIEW B **100**, 144105 (2019)

Editors' Suggestion

Machine-learning interatomic potential for radiation damage and defects in tungsten

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$$E_i = \underbrace{\frac{1}{2}\sum_j E_{\text{rep.}}(r_{ij})}_{\text{Repulsive pair potential}} + \underbrace{\sum_s \alpha_s^{2\text{b}} K_{2\text{b}}(\boldsymbol{q}_i, \boldsymbol{q}_s)}_{\text{ML pair potential}} + \underbrace{\sum_s \alpha_s^{\text{mb}} K_{\text{mb}}(\boldsymbol{q}_i, \boldsymbol{q}_s)}_{\text{ML many-body potential}}$$

PHYSICAL REVIEW MATERIALS **4**, 093802 (2020)

Gaussian approximation potentials for body-centered-cubic transition metals

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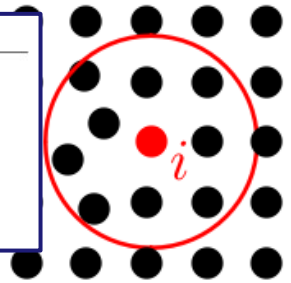
Potential energy

Interatomic distance



J. Byggmästar, A. Hamedani, K. Nordlund, and F. Djurabekova, Phys. Rev. B, **100**, 144105 (2019)
J. Byggmästar, K. Nordlund, and F. Djurabekova, Phys. Rev. Materials, **4**, 093802 (2020)

tabGAP: tabulated low-dimensional GAPs

- Tabulate GAP predictions → cubic spline interpolations
- Any combination of low-dimensional descriptors:
  - Two-body (pairs)
  - Three-body (triplets)
  - Many-body: EAM-like density $\rho_i = \sum_j \varphi(r_{ij})$

GAP:

$$E = \sum_{ij}^{N} E_{\text{ext.}}(r_{ij}) + \sum_{ij}^{N}\sum_{s}^{M_{2b}} \alpha_s K_{2b}(\boldsymbol{q}_i, \boldsymbol{q}_s) + \sum_{ijk}^{N}\sum_{s}^{M_{3b}} \alpha_s K_{3b}(\boldsymbol{q}_i, \boldsymbol{q}_s) + \sum_{i}^{N}\sum_{s}^{M_{EAM}} \alpha_s K_{EAM}(\boldsymbol{q}_i, \boldsymbol{q}_s)$$

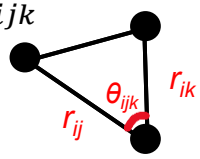
Pair potential: 1D grid

3-body potential: 3D grid

EAM embedding energy: two 1D grids

tabGAP:

$$E = \sum_{ij}^{N} S_{1D}(r_{ij}) + \sum_{ijk}^{N} S_{3D}(r_{ij}, r_{ik}, \cos\theta_{ijk}) + \sum_{i}^{N} S_{1D}(\rho_i), \qquad \rho_i = \sum_j s_{1D}(r_{ij})$$

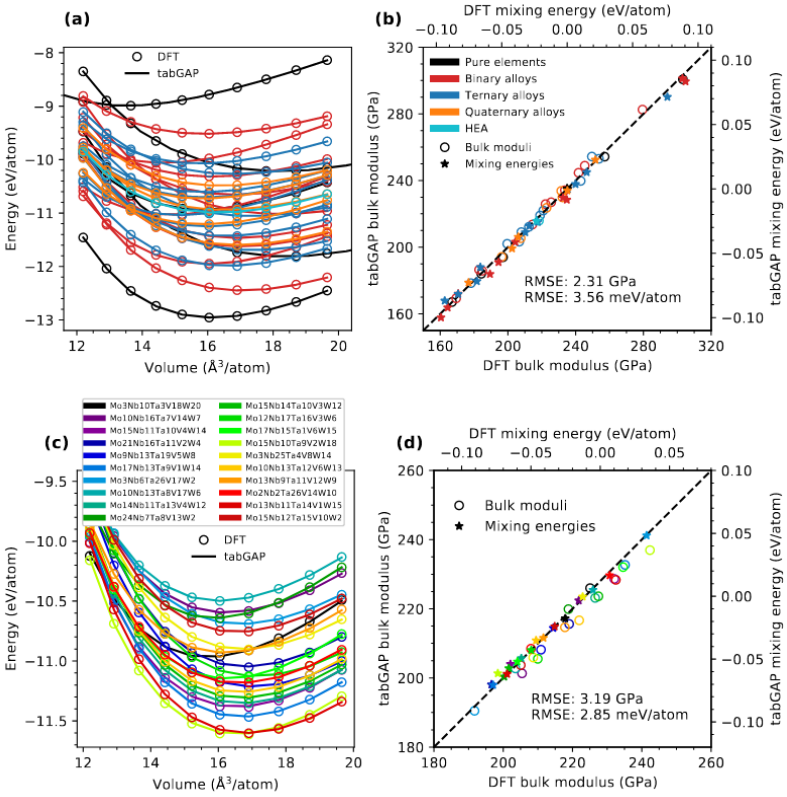


Normal EAM embedding function

Similar work:
- [A. Glielmo, C. Zena, A. De Vita, PRB 97 (2018)]
- FLARE https://github.com/mir-group/flare (J. Vandermause, et al.)

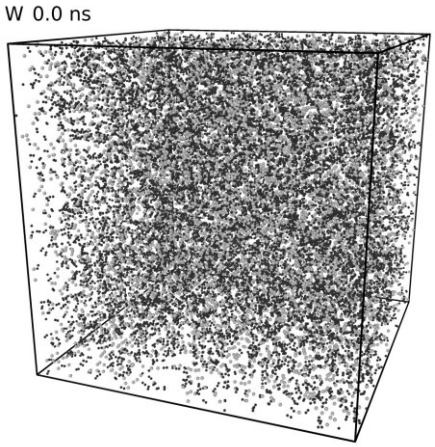
tabGAP for Mo-Nb-Ta-V-W alloys

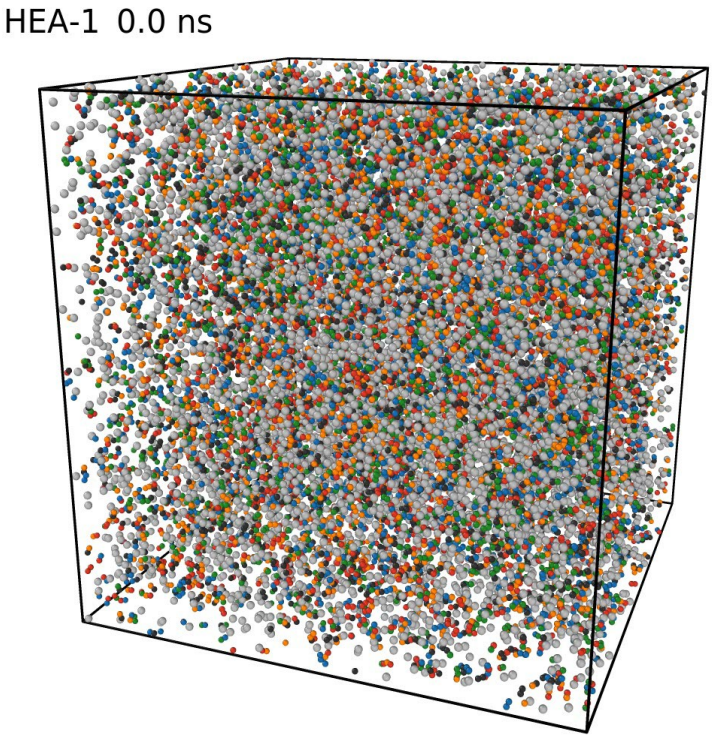
- We have developed a few tabGAP potentials including the high entropy alloys
- Comparison of DFT and tabGAP predictions for energy per atom as a function of atomic volume,
  - a) for all equiatomic compositions for pure, binary, ternary, quaternary and HEA alloys, while in c) the alloy compositions sampled randomly
  - b) and d) bulk moduli and mixing energies deduced from the curves in a) and c), respectively.



[J. Byggmästar, K. Nordlund, and F. Djurabekova PRB 104, 104101 (2021)]

Defect annealing W vs. HEA



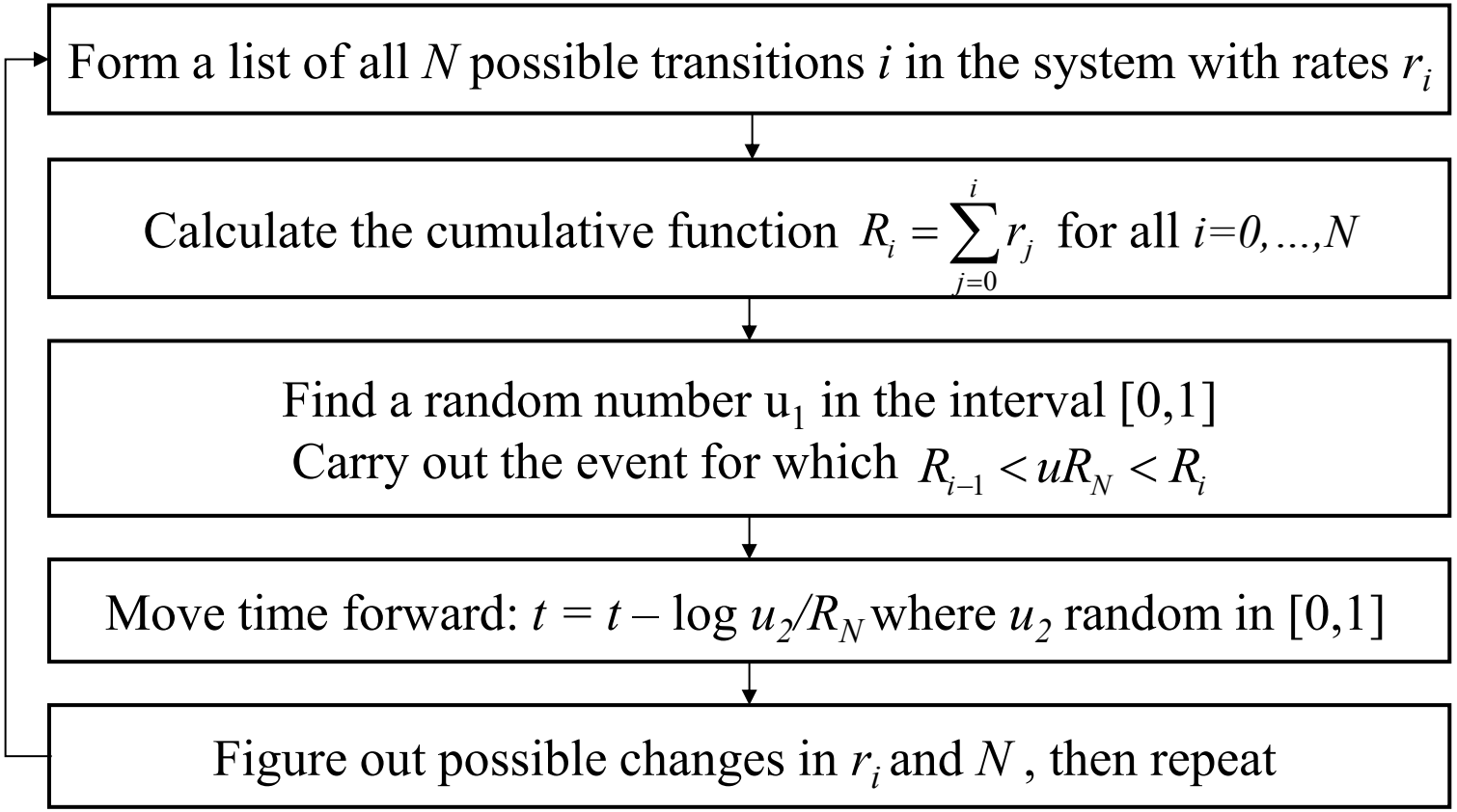


[J. Byggmästar, K. Nordlund, and F. Djurabekova PRB 104, 104101 (2021)]

Long-term relaxation of defects - How to model that?

- Multibody collisions are well covered by MD
  - However, the time span of MD is heavily limited
  - Many defects which form initially in cascades have long time to relax before the next collisional cascades hits at the same spot
- The long-time-scale relaxation phase after the collisional stage can take microseconds, seconds, days or years
  - Microseconds to seconds important in semiconductors
  - Years important in nuclear fission and fusion reactor materials
- Several groups, including us, have recently taken into use Kinetic Monte Carlo (KMC) to be able to handle all this
  - Also rate theory (numerical solution of differential equations) can be extremely useful in this regard

Kinetic Monte Carlo (the residence-time algorithm)



Comments on KMC algorithm

- The KMC algorithm is actually exactly right for so-called Poisson processes, i.e. processes occurring independent of each other at constant rates
  - *Stochastic but exact*
- Typical use:
  - Atom diffusion: rates are simply atom jumps
- But how to know the input rates r_i ?
  - The algorithm itself can't do anything to predict them
  - I.e. they have to be known in advance somehow
- From experiments, DFT simulations, …
- Also knowing reactions may be difficult
- Many varieties of KMC exist: object KMC, lattice object KMC, lattice all-atom KMC, …
  - For more info, see wikipedia page on KMC

Principles of object KMC for defects

- Basic object is an impurity or intrinsic defect in lattice
  - Non-defect lattice atoms are not described at all!
- Basic process is a diffusive jump, occurring at Arrhenius rate

$$r_i = r_0 e^{-E_A / k_B T}$$

- Incoming ion flux can be easily recalculated to a rate!
- But also reactions are important: for example, formation of a divacancy from two monovacancies, or a pair of impurities
- Reactions typically are dealt with by using a simple recombination radius:
  - if species A and B are closer than some recombination radius r_{AB}, they instantly combine to form defect complex

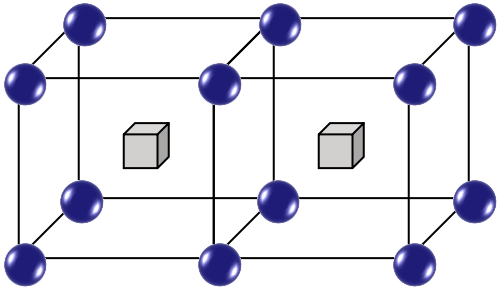
Di-vacancy in a monoatomic lattice

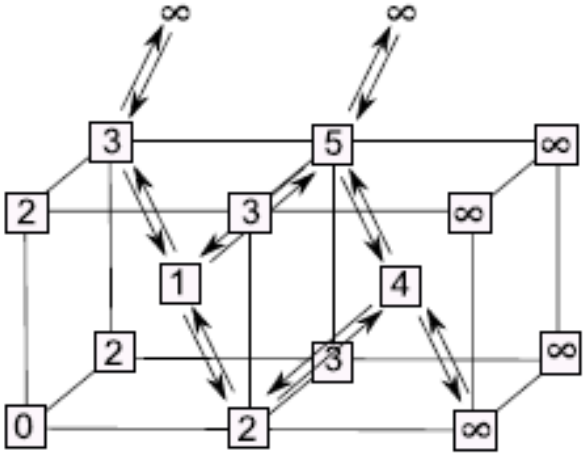
- We consider the only one empty site to affect the barrier for the vacancy migration
- Even this simpliest case will result in a number of barriers.
- These can be described as a linear relationship with energy variation (Metropolis-like approach)

$$E_a = E_0 + \frac{E_f - E_i}{2}$$

$$E_0 = \text{constant}$$

- Or calculated explicitly as a function of local atomic environment (LAE)

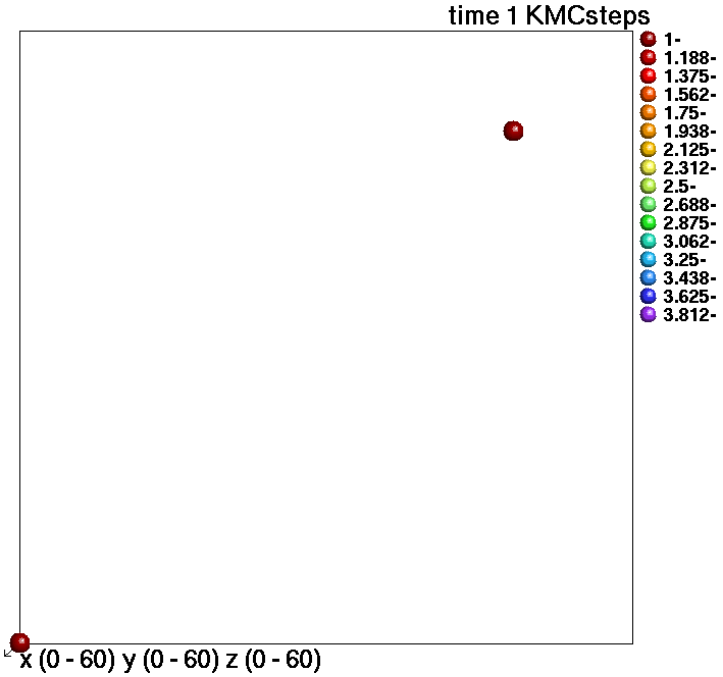




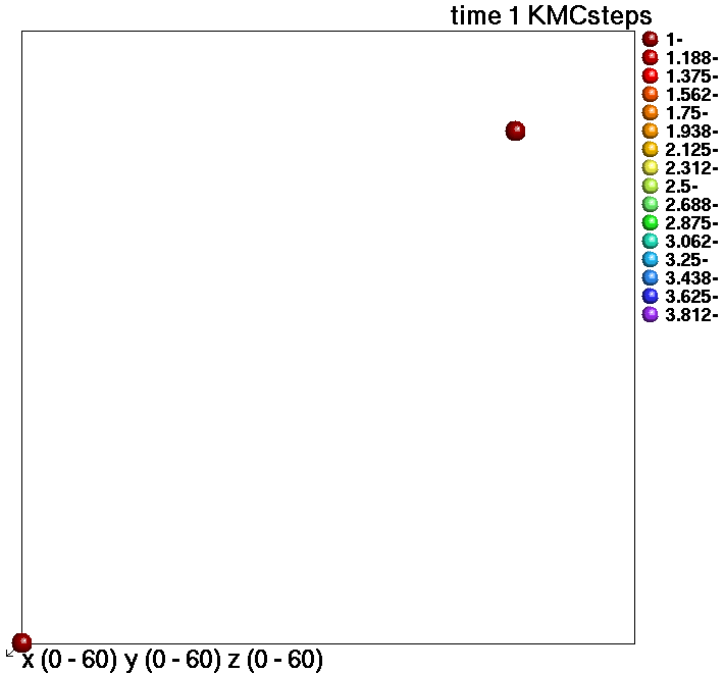
KMC simulation of divacancies in the lattice KMC model (lakimoca)

- Using Metropolis-like approach, we observe mostly 2nn-1nn jumps, while the calculated barriers using empirical interatomic potentials (drag method), the jumps are 2nn-4nn

LAE dependent barrier method

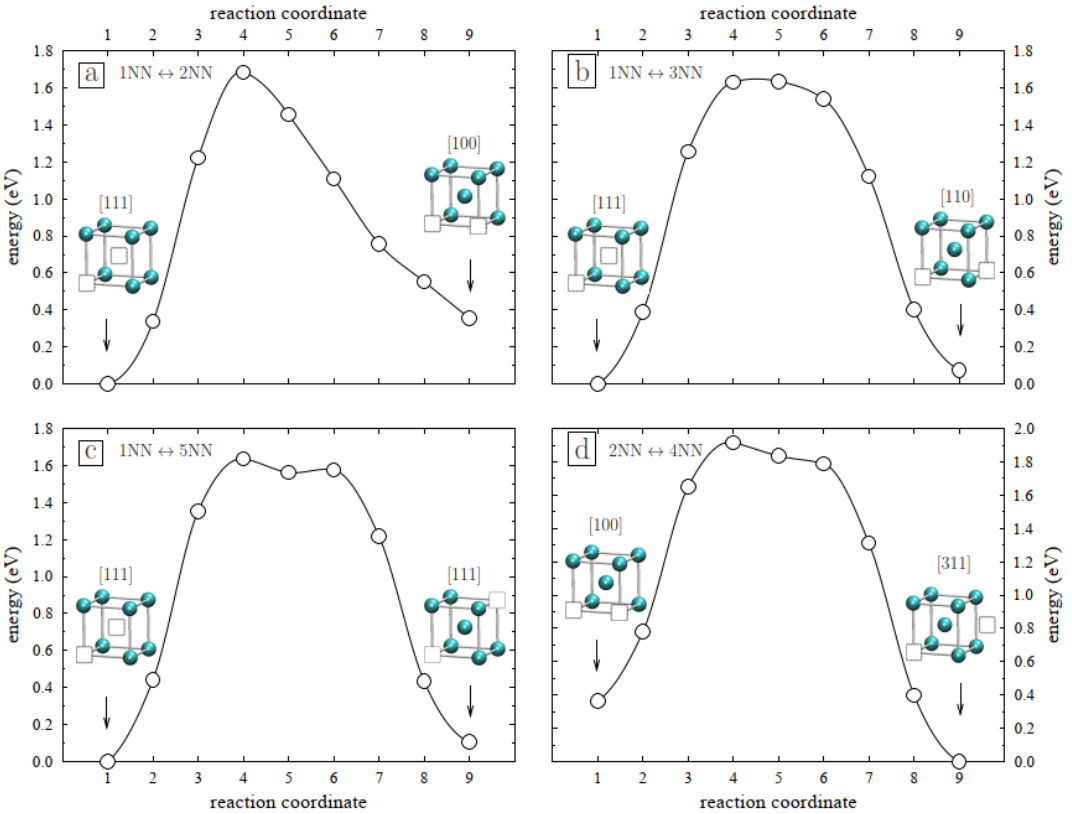


Metropolis-type method



[F. Djurabekova, L. Malerba, R. C. Pasianot, P. Olsson, and K. Nordlund, Philosophical Magazine 90, 2585 (2010)]

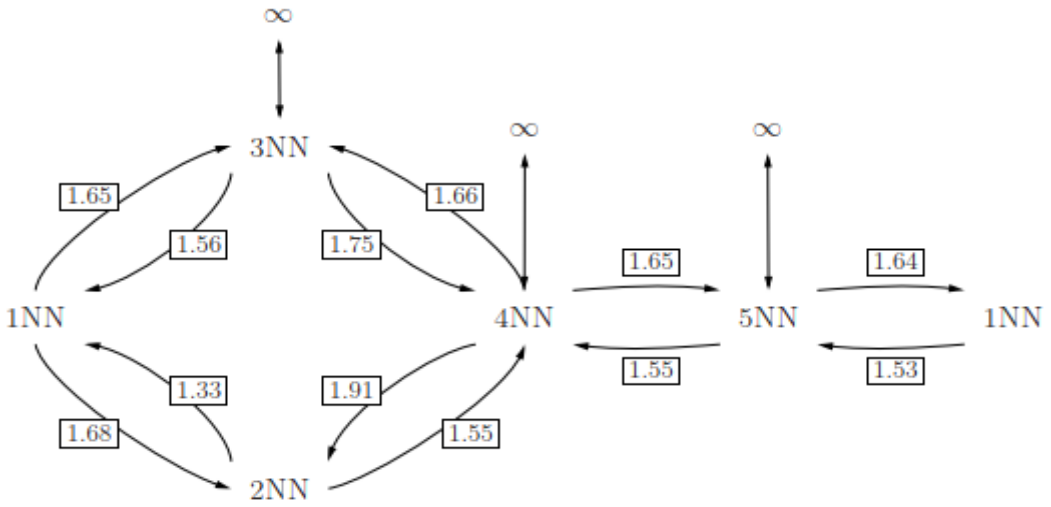
Calculating the barriers



- More accurate way to assess the barriers is to use the NEB calculations, where a few replicas are relaxed together to find the minimum energy path

[K. Heinola, F. Djurabekova, and T. Ahlgren, Nuclear Fusion, 58 (2018) 026004]

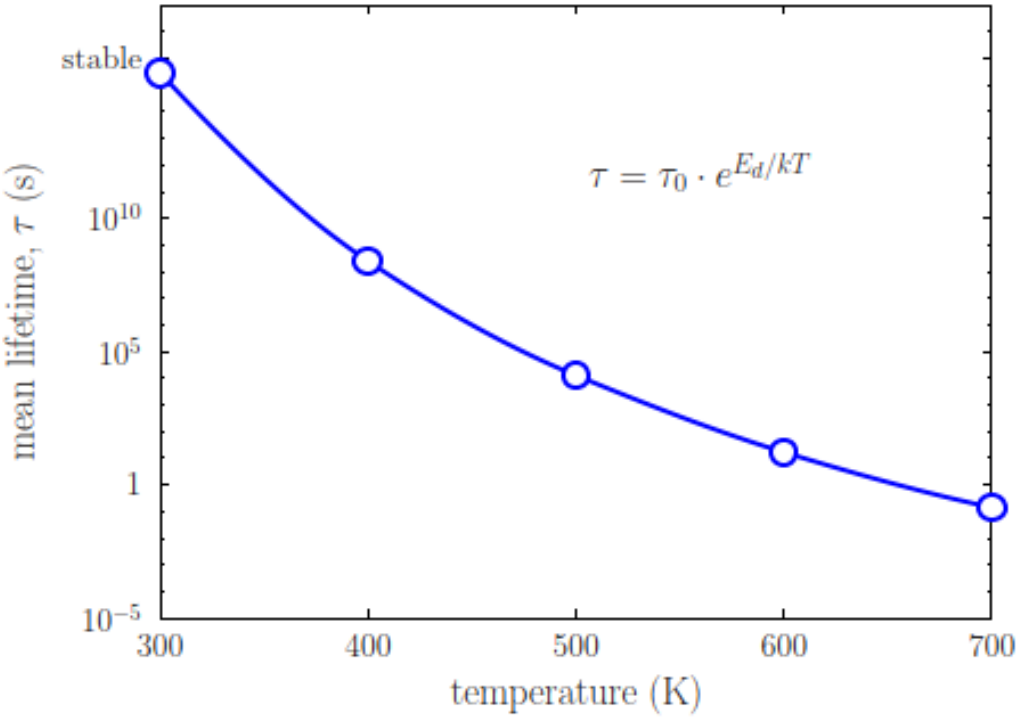
Migration paths



- In the current calculations, only 1NN and 4NN yielded in the bounds states: $E_b^{1NN} = 0.01$ eV; $E_b^{4NN} = 0.02$ eV,
- 2NN, 3NN and 5NN have negative binding energies: $-0.035, -0.07$ and -0.1 which is explained by density of states at Fermi level in specific configurations

[K. Heinola, F. Djurabekova, and T. Ahlgren, Nuclear Fusion, 58 (2018) 026004]

Bound states for divacancies in W



- Despite small binding energies, the di-vacancies can be stable up to rather high temperatures because of the high dissociation barriers

[K. Heinola, F. Djurabekova, and T. Ahlgren, Nuclear Fusion, 58 (2018) 026004]

Binding energies of vacancy-C complexes (eV)

$AB \longrightarrow A + B$		E_b
$V_1C_1 \longrightarrow$	$V_1 + C_1$	2.05
$V_2^{2NN}C_1 \longrightarrow$	$V_1C_1 + V_1$	1.29
	$V_2^{1NN} + C_1$	3.33
	$V_2^{2NN} + C_1$	3.69
$V_2^{1NN}C_1 \longrightarrow$	$V_1C_1 + V_1$	0.04
	$V_2^{1NN} + C_1$	2.08
	$V_2^{2NN} + C_1$	2.44

- Similarly to H impurities, C also can stabilize divacancies in W.
- Different V_2-impurity dissociation channels shown for the first (1NN) and second (2NN) nearest neighbour V_2 configurations.
  - The data shows that $V_2^{2NN}C_1$ is the most stable complex up to very high temperatures

[K. Heinola, F. Djurabekova, and T. Ahlgren, Nuclear Fusion, 58 (2018) 026004]

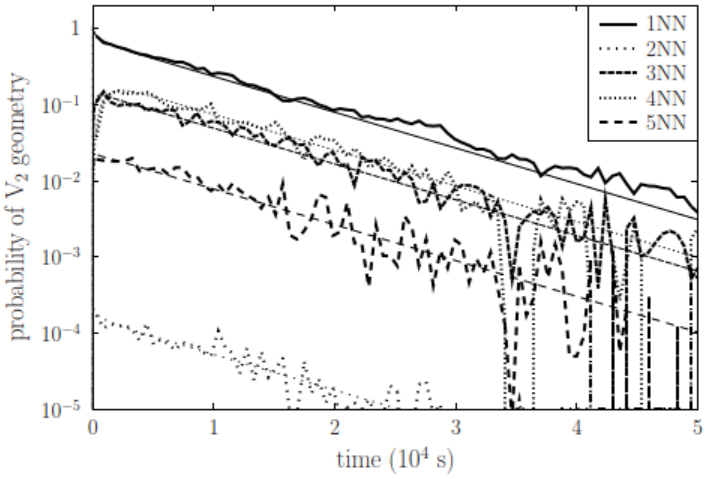
Solving Master equations!

$$\begin{cases} \frac{dC_1}{dt} = K^{21}\cdot C_2 + K^{31}\cdot C_3 + K^{51}\cdot C_5 \\ \qquad -(K^{12}+K^{13}+K^{15})\cdot C_1 \\ \frac{dC_2}{dt} = K^{12}\cdot C_1 + K^{42}\cdot C_4 - (K^{21}+K^{24})\cdot C_2 \\ \frac{dC_3}{dt} = K^{13}\cdot C_1 + K^{43}\cdot C_4 - (K^{31}+K^{34}+K^{3\infty})\cdot C_3 \\ \frac{dC_4}{dt} = K^{24}\cdot C_2 + K^{34}\cdot C_3 + K^{54}\cdot C_5 \\ \qquad -(K^{42}+K^{43}+K^{45}+K^{4\infty})\cdot C_4 \\ \frac{dC_5}{dt} = K^{15}\cdot C_1 + K^{45}\cdot C_4 - (K^{51}+K^{54}+K^{5\infty})\cdot C_5 \end{cases}$$

$$K^{ij} = k_{ij}\Gamma_{ij} = k_{ij}\nu_0 \exp\left(-\frac{E_{ij}^m}{k_B T}\right)$$

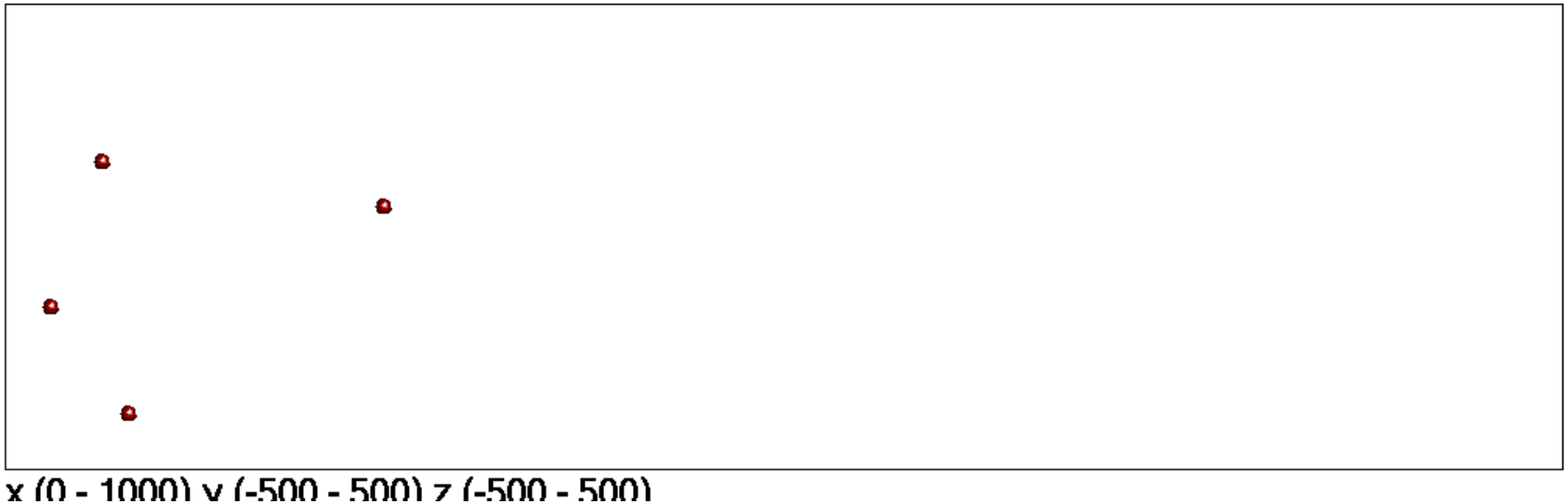
[K. Heinola, F. Djurabekova, and T. Ahlgren, Nuclear Fusion, 58 (2018) 026004]

- Solving Master equations that include all formation and dissociation reactions can help to see more prominent states in the system at given temperature
- Figure to the right shows the agreement between KMC and PDE



Example animation

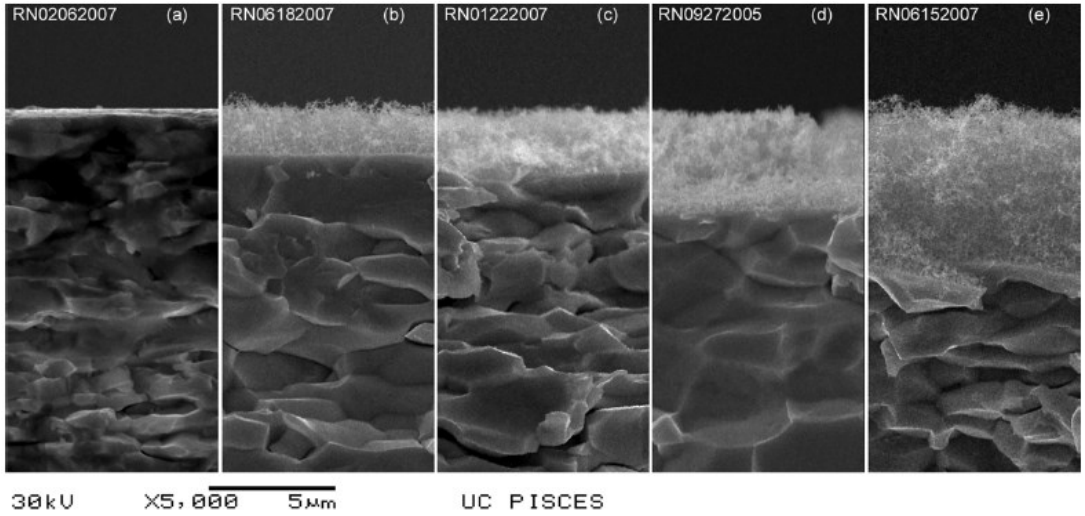
- Simple fusion-relevant example: He mobility and bubble formation in W
  - Inputs: experimental He migration rate, experimental flux, recombination radius of 3 Å, clusters assumed immobile



[K. O. E. Henriksson, **K. Nordlund**, A. Krasheninnikov, and J. Keinonen, Fusion Science & Technology **50**, 43 (2006).]

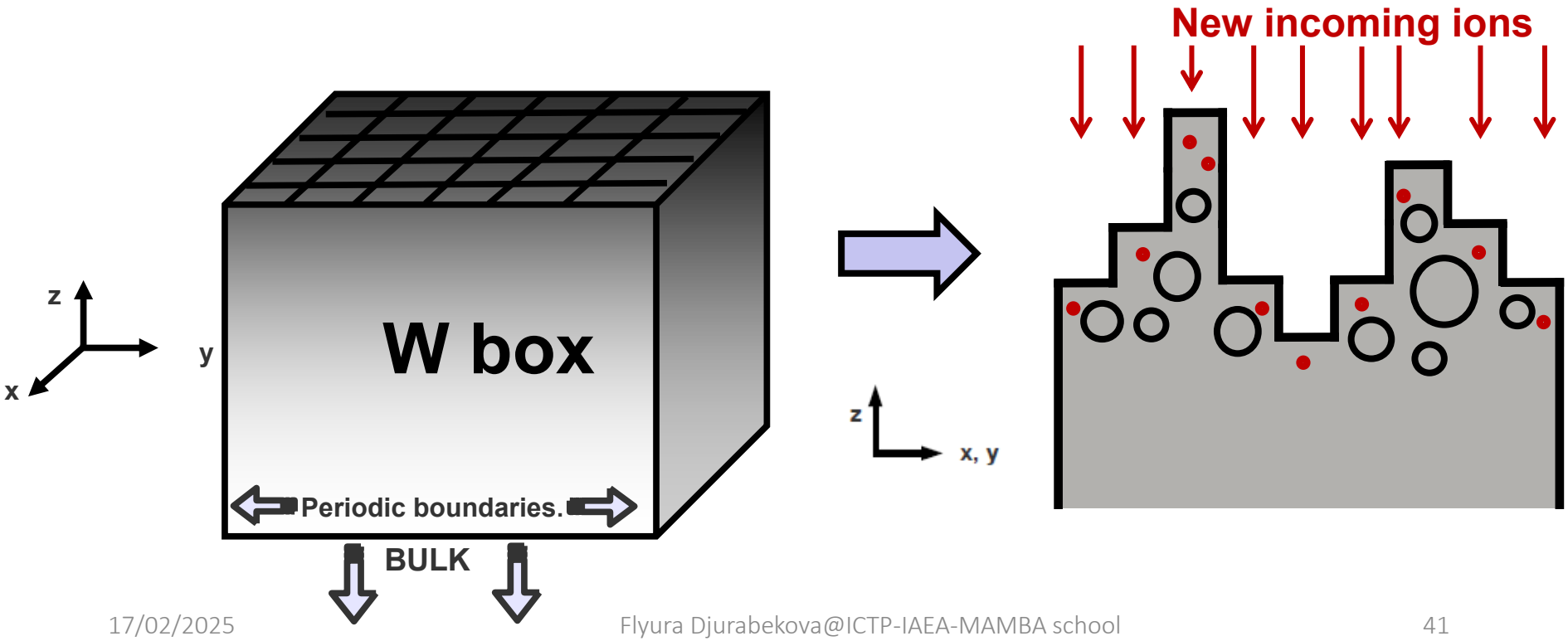
Advanced fusion-relevant example: fuzz growth by He on W irradiation

- In 2008 Baldwin and Doerner at UCSD showed with a linear plasma machine that W when irradiated by ~ 100 eV He (typical fusion reactor energy) forms a highly underdense porous layer
  - Often called ‘fuzz’ due to visual impression
  - Forms in 900 – 2000 K temperature interval
- Could be very harmful in fusion reactors:
  - Enhances electrical arcing
  - Wall properties change



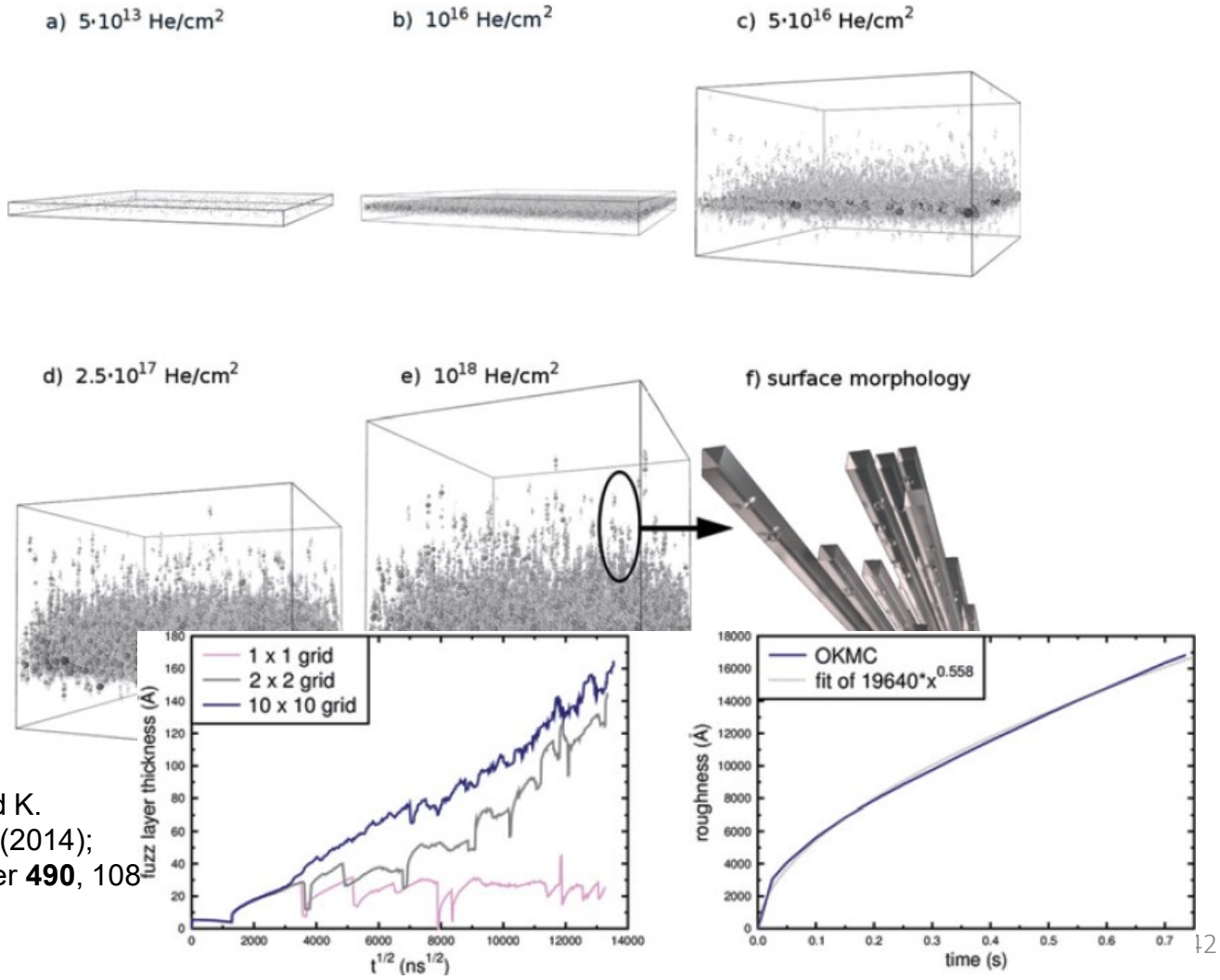
Development of fuzz KMC model

- These observations from MD were used to develop a new Object KMC model
- Basic objects: mobile He, trapped He, He in bubbles
- Simulation cell made to have a variable height h(x,y) on a grid



Fuzz formation from OKMC

- N

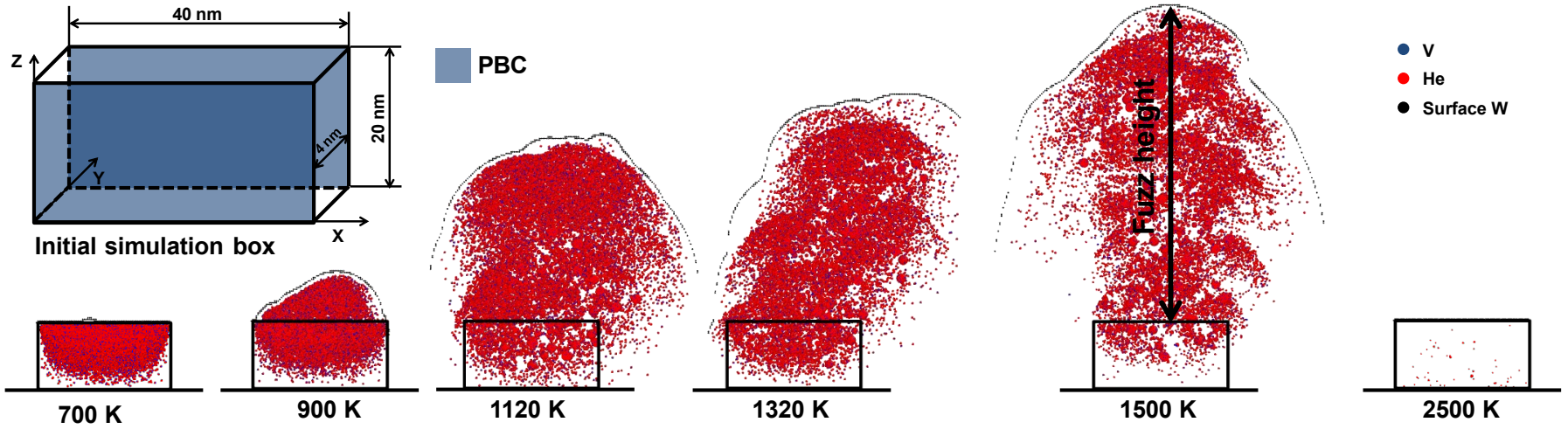


[A. Lasa, S. K. Tähtinen and K. Nordlund, EPL 105, 25002 (2014); G. Valles et al, J. Nucl. Mater **490**, 108 (2017).]

Fuzz formation from OKMC with more complex objects (MMonCa)

- Temperature dependence is similar to experiments!

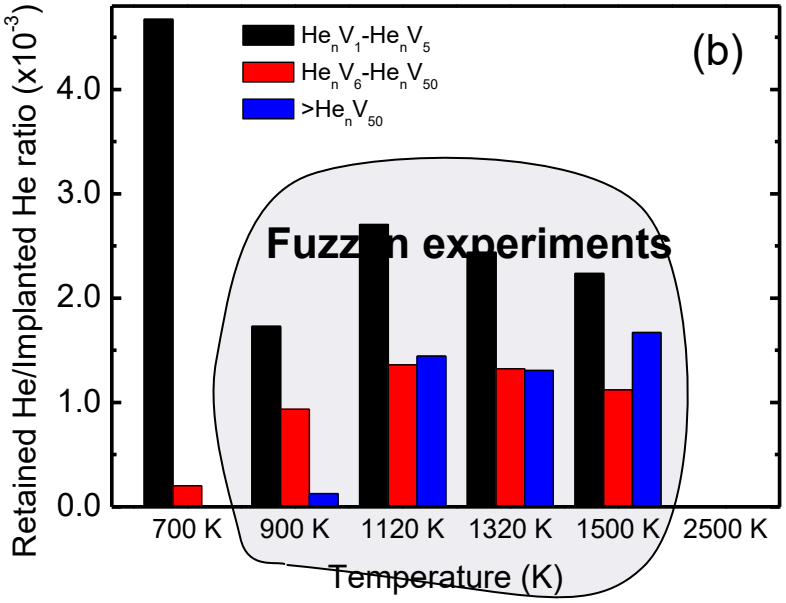
$$E_b(He \rightarrow He_{n-1}V_m) = 4.43 \cdot \left(\frac{n}{m}\right)^{-0.28}$$



[A. Lasa, S. K. Tähtinen and K. Nordlund, EPL 105, 25002 (2014);
G. Valles et al, J. Nucl. Mater **490**, 108 (2017).]

Why the T dependence?

- We analyzed the T dependence in detail
- The crucial factor is the clustering:
  - At high T all He detrap and no bubbles form
    - ⇨ This is pretty obvious
  - At low T detailed analysis showed that almost all He stays in single-vacancy clusters as He_9V_1 and no large clusters form



Summary

- Multiscale modelling is the only approach to cover all stages of damage evolution in the system
- Monte Carlo based methods give a versatile alternative to the deterministic methods also in studies of behavior of materials under extreme environments
- However, for more accurate atomic dynamics, the Molecular Dynamics methods are still preferred
  - One has to be very precise with setting the input parameters to ensure that numerical integration does not make your system explode!
- Kinetic Monte Carlo estimates the residence time needed for each process in the system to ripe up and take place. The competition of different processes may result in unexpected results!

The 24th international conference on Ion Beam Modification of Materials IBMM24

21 – 26 June 2026

@University of Helsinki
Finland

- Organizers:
  - Flyura Djurabekova
  - Kai Nordlund
  - Filip Tuomisto
  - Kostas Sarakinos

- Scope:
  - The scope of the conference ranges from fundamental radiation materials science to industry applications.
  - Physicists, chemists, material scientists, engineers, and anybody who is interested in the use of ion beams for surface and material modification in their research and/or industrial application are welcome!

Thank you for your attention!

Questions?

Working with CERN, ITER, EUROFusion, FAIR, ORNL, LLNL, …

Results since 1998:

- **~ 600 publications**
- **43 PhD theses**