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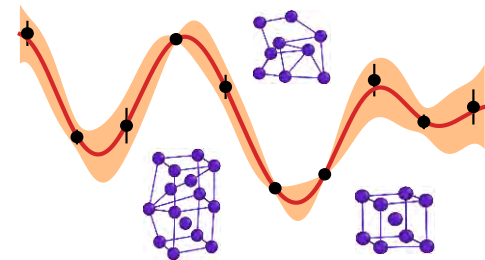
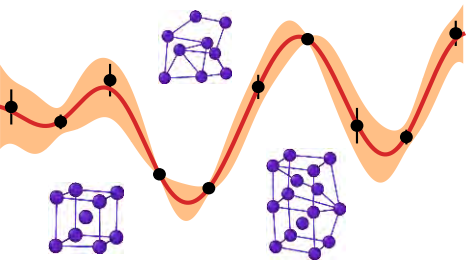
**FCAI**



# Machine-learned interatomic potentials for atomistic simulations of fusion materials

**Jesper Byggmästar**

*Department of Physics, University of Helsinki*



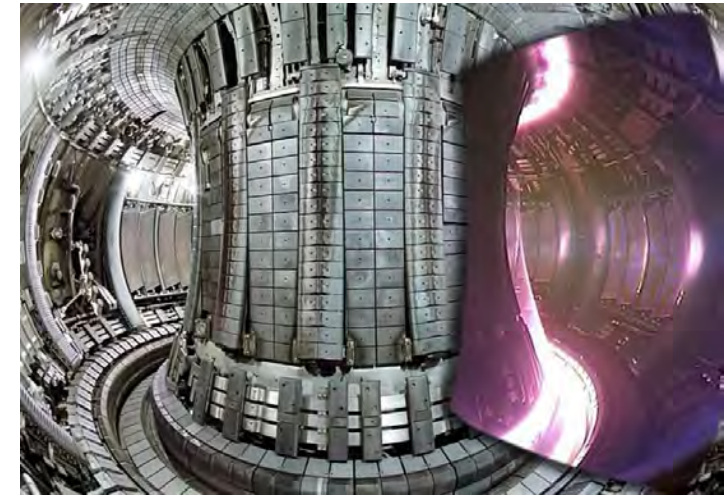


# Outline

- Fusion reactor materials
- High-entropy alloys
- Machine learning for molecular dynamics simulations
- Highlights of results and ongoing work
  - Large-scale simulations of irradiation and plasticity



# Fusion reactor materials

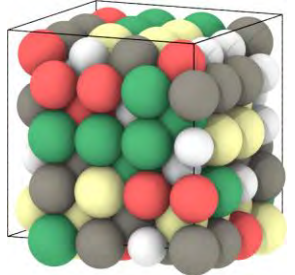


Periodic table of the elements

group 1*		group 2												group 13-18																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
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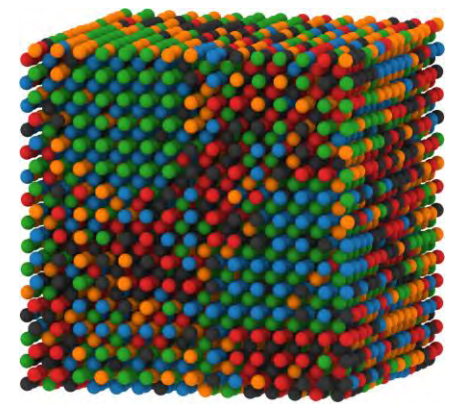
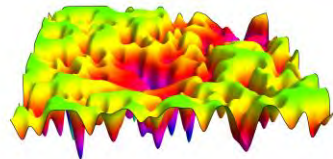
\*Numbering system adopted by the International Union of Pure and Applied Chemistry (IUPAC). © Encyclopædia Britannica, Inc.

- Tungsten
  - H, He, Re, Os
- High-entropy alloys?
  - Better irradiation tolerance?
    - Both neutron and light-ion?
  - Better (low-*T*) ductility?

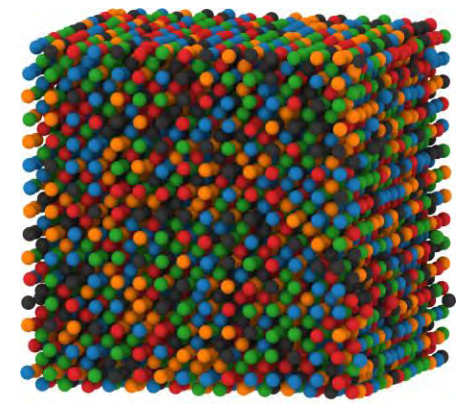




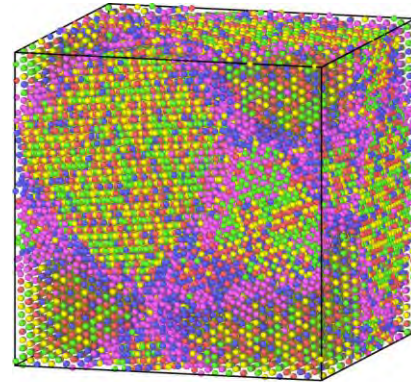
# High-entropy alloys



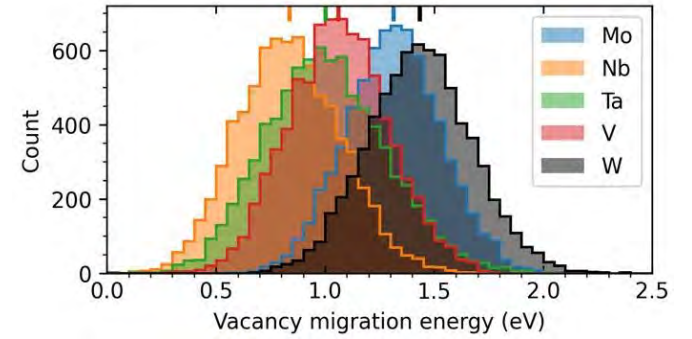
300 K



1000 K

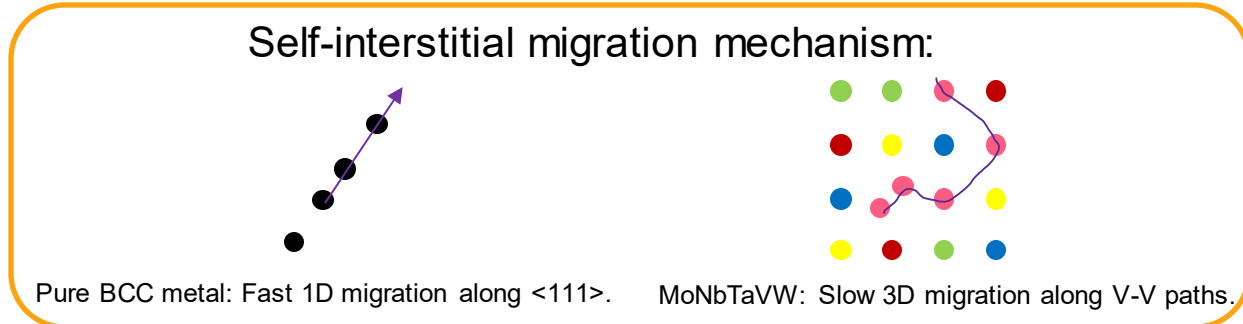


MoNbTa V W  
Particle types



➤ Mix of many elements leads to complex inhomogeneous potential energy landscape, consequences:

- Lattice distortion
- Order or disorder?  $G = H - TS$
- Segregation
- Wide distributions of defect energies
- Different migration mechanisms
- **Still gaps in fundamental understanding of above list!**

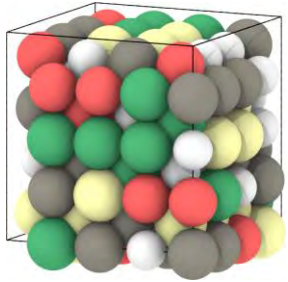


# Molecular dynamics simulations



## ➤ Classical molecular dynamics

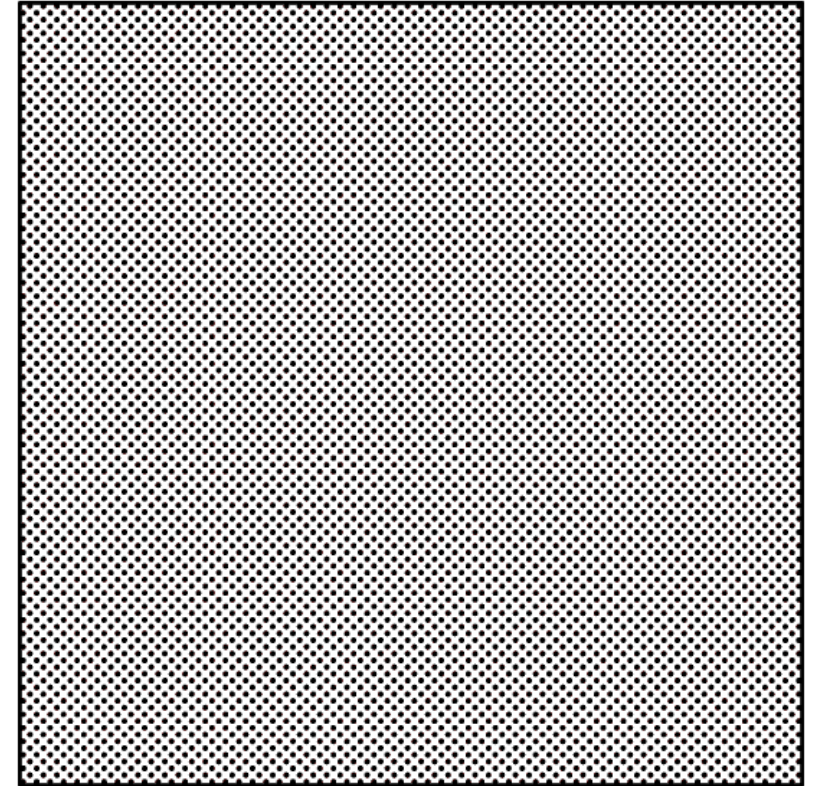
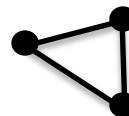
- Newton's equations of motion atom by atom
- Atoms interact with some *interatomic potential*,  $V$



$$\mathbf{F}_i = -\nabla_i V.$$

Formally, can expand it as a material-dependent many-body cluster expansion:

$$V = V_0 + \sum_i V_1(\mathbf{r}_i) + \frac{1}{2} \sum_{ij} V_2(\mathbf{r}_i, \mathbf{r}_j) + \frac{1}{3!} \sum_{ijk} V_3(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) + \dots$$





# Machine-learning interatomic potentials

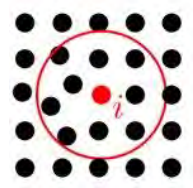
Do:

- Express total energy as sum of local energies

$$E_{\text{tot}} = \sum_i E_i$$

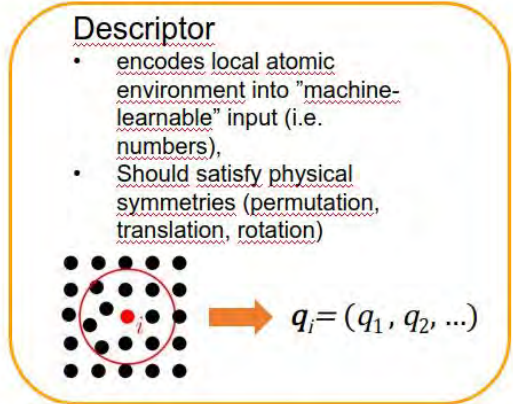
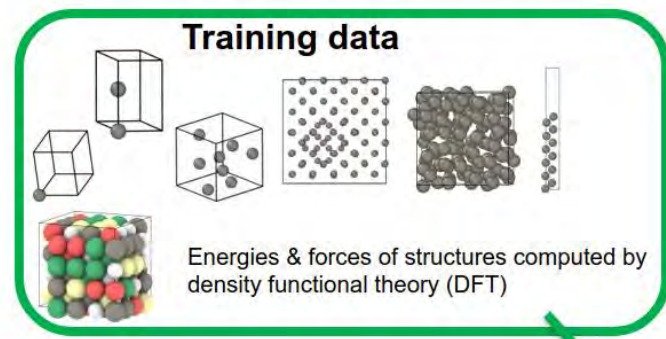
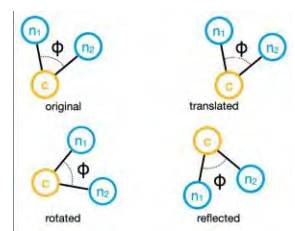
Assume:

- Locality:** atoms only interact with others within some cutoff radius (pre-defined, material-dependent).

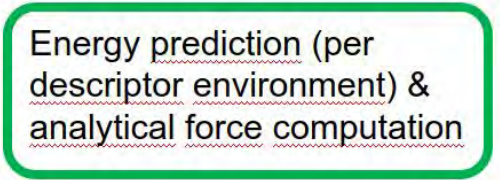


Consider:

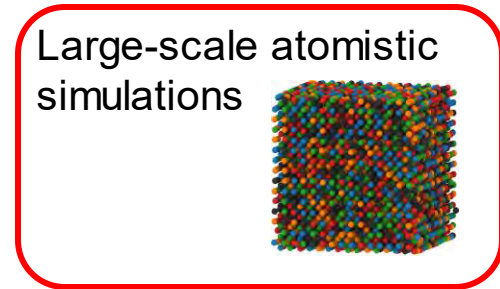
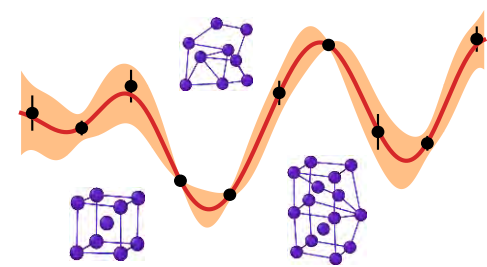
- Physical symmetries:** invariant to translation, rotation, permutation.



$$E_{\text{tot}} = \sum_i E_i = \sum_i f_{\text{ML}}(q_i)$$



- Function, linear regression, kernel/Gaussian process regression, artificial neural network, ...





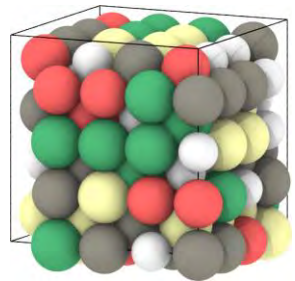
# Simple machine-learned interatomic potentials

$$V = V_0 + \sum_i V_1(\mathbf{r}_i) + \frac{1}{2} \sum_{ij} V_2(\mathbf{r}_i, \mathbf{r}_j) + \frac{1}{3!} \sum_{ijk} V_3(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) + \dots$$

- Most ML potentials use "complex" (many-body, high-dimensional) descriptors.
  - Flexible, high accuracy, but slow and not necessarily good for (chemically) complex materials!



- **tabGAP**: Complex many-element alloys? Use simple descriptors (low-body, low-dimensional), with robust regression method (Gaussian process regression)!

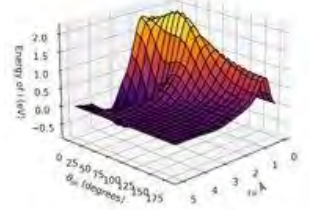
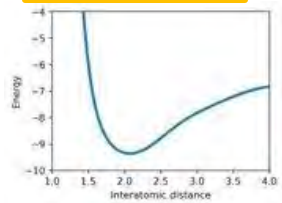


$$E = \sum_{ij}^N S_{1D}(r_{ij}) + \sum_{ijk}^N S_{3D}(r_{ij}, r_{ik}, \cos \theta_{ijk}) + \sum_i^N S_{1D}(\rho_i), \quad \rho_i = \sum_j S_{1D}(r_{ij})$$

**2-body**

**3-body**

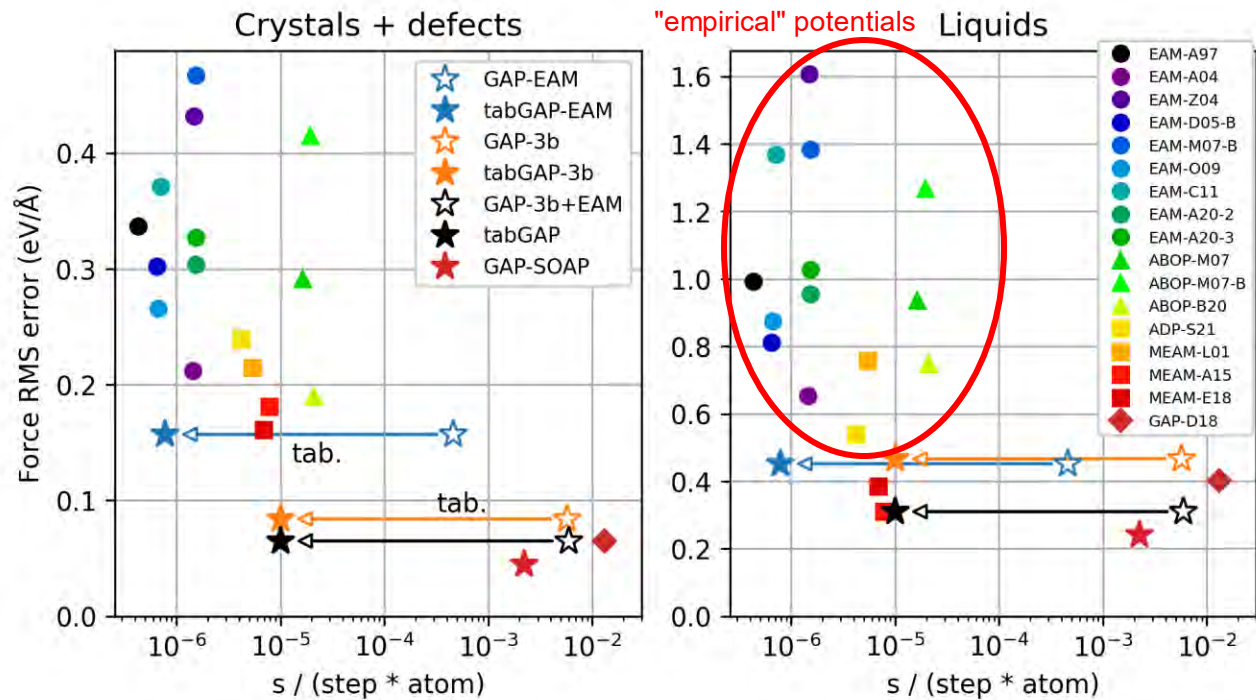
**simple many-body**



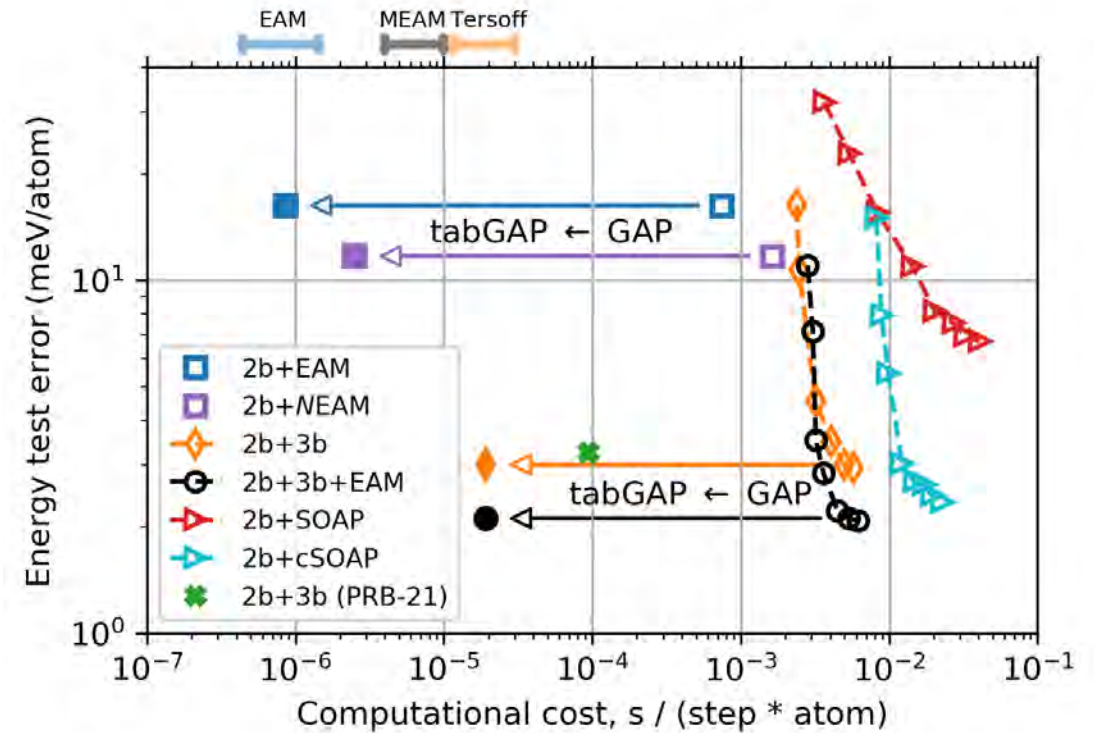


# Computational cost? Cheap!

Fe



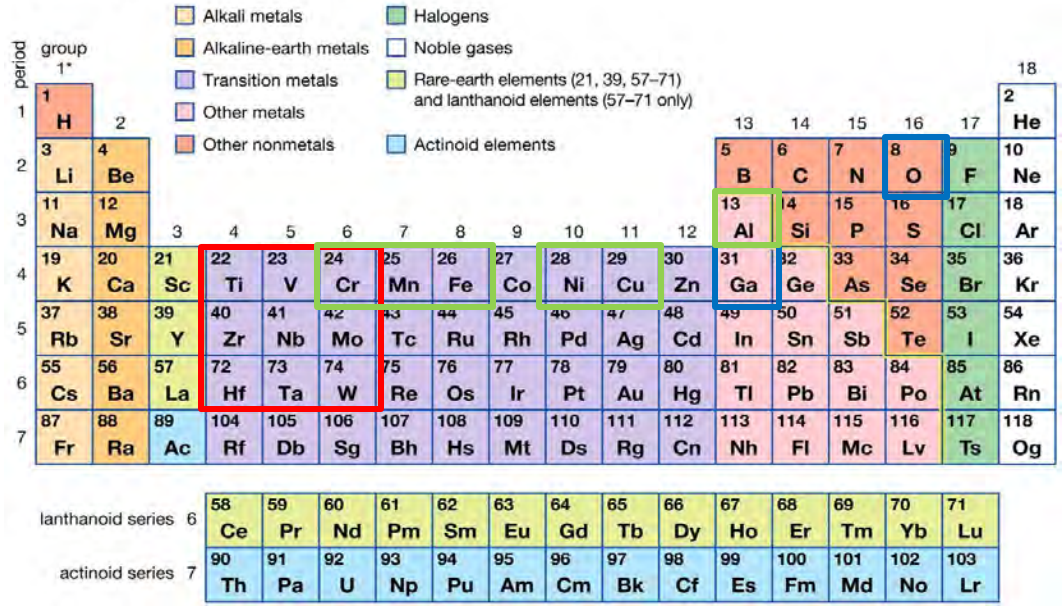
Mo-Nb-Ta-V-W



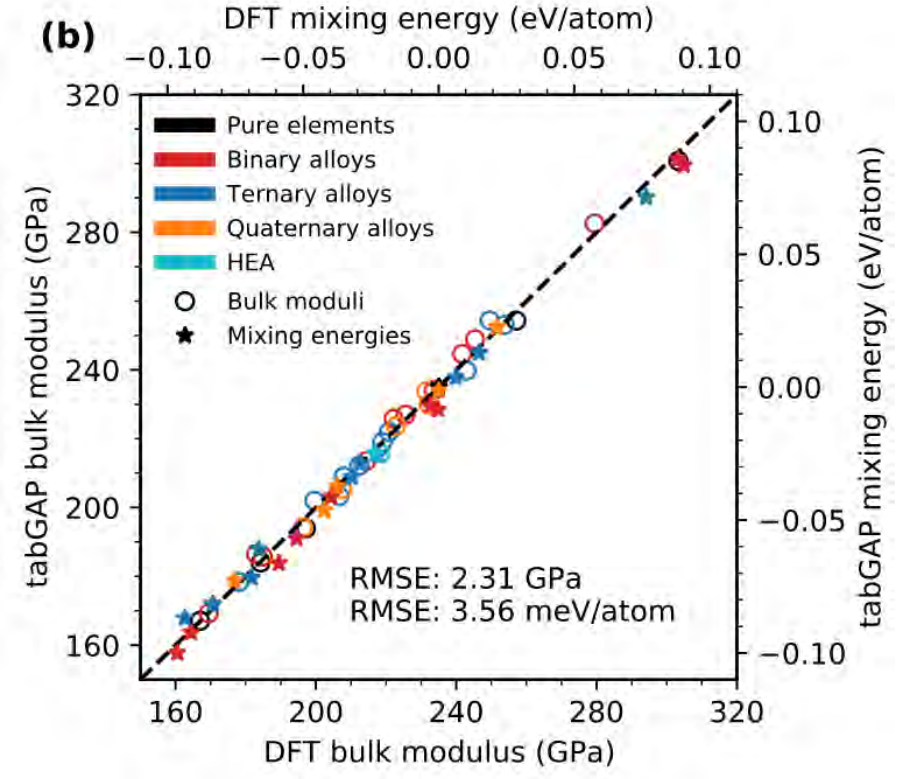


# Simple machine-learned interatomic potentials

Periodic table of the elements



\*Numbering system adopted by the International Union of Pure and Applied Chemistry (IUPAC). © Encyclopædia Britannica, Inc.

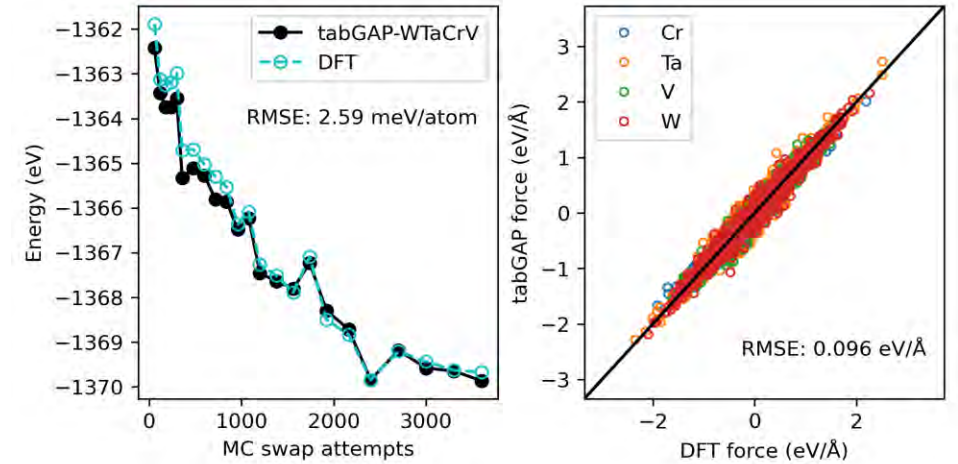
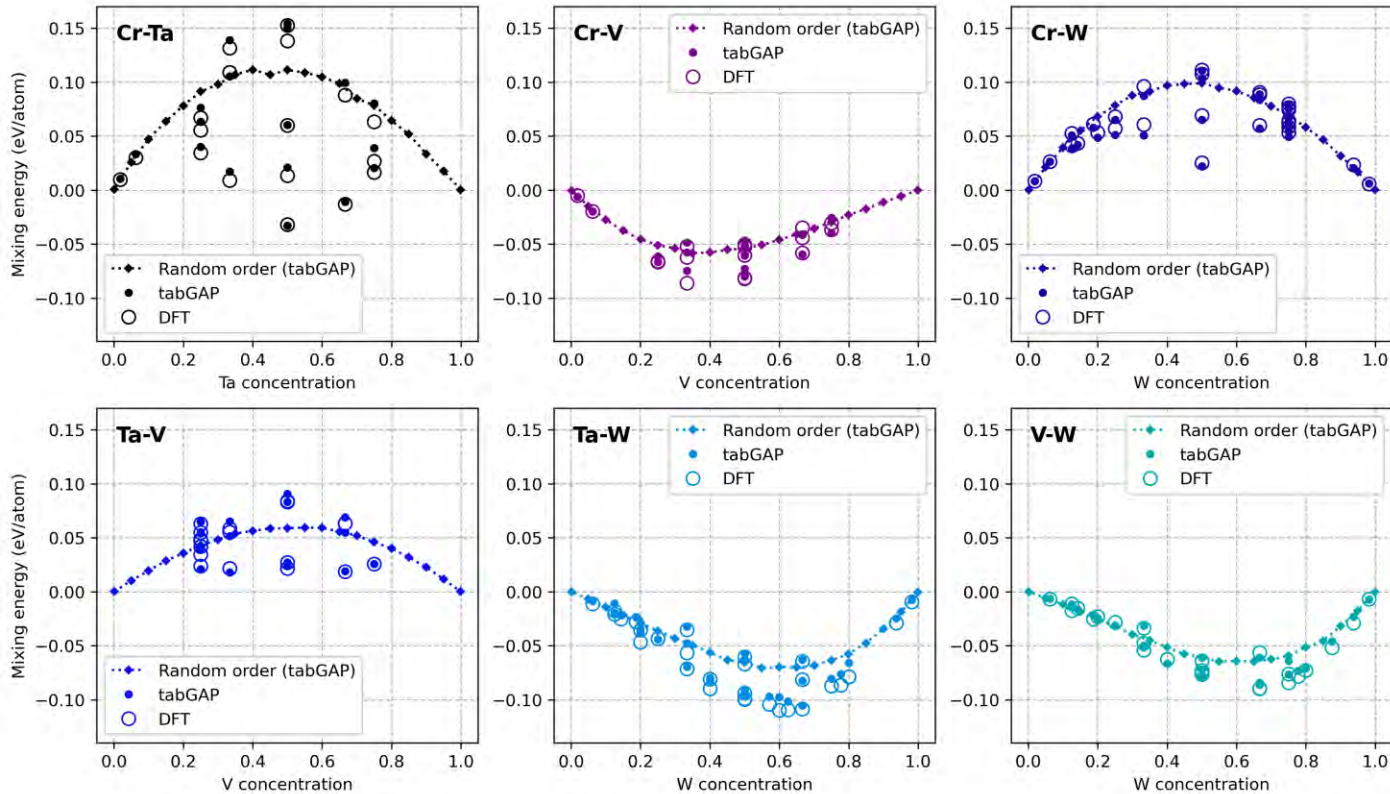


- **JB**, K. Nordlund, and F. Djurabekova, *Phys Rev. Materials* 6, 083801 (2022)
- **JB**, G. Nikoulis, A. Fellman, K. Nordlund *et al* 2022 *J. Phys.: Condens. Matter* **34** 305402
- Junlei Zhao, **JB**, H. He, F. Djurabekova, *et al* *npj Computational Materials* **9**, 159 (2023)
- A. Fellman, **JB**, F. Granberg, F. Djurabekova, K. Nordlund, *et al.* (in preparation)

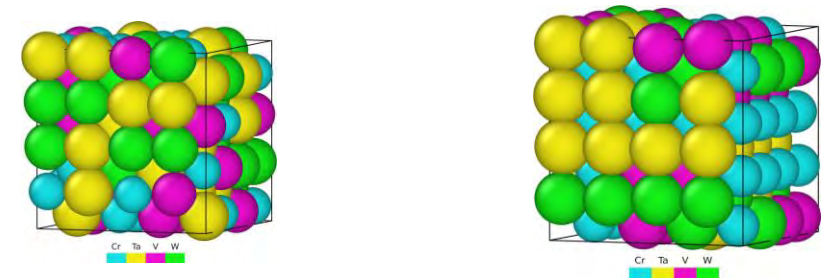


# Machine-learning potentials for alloys: validation

## Enthalpy of mixing, binary alloys of W-Ta-Cr-V



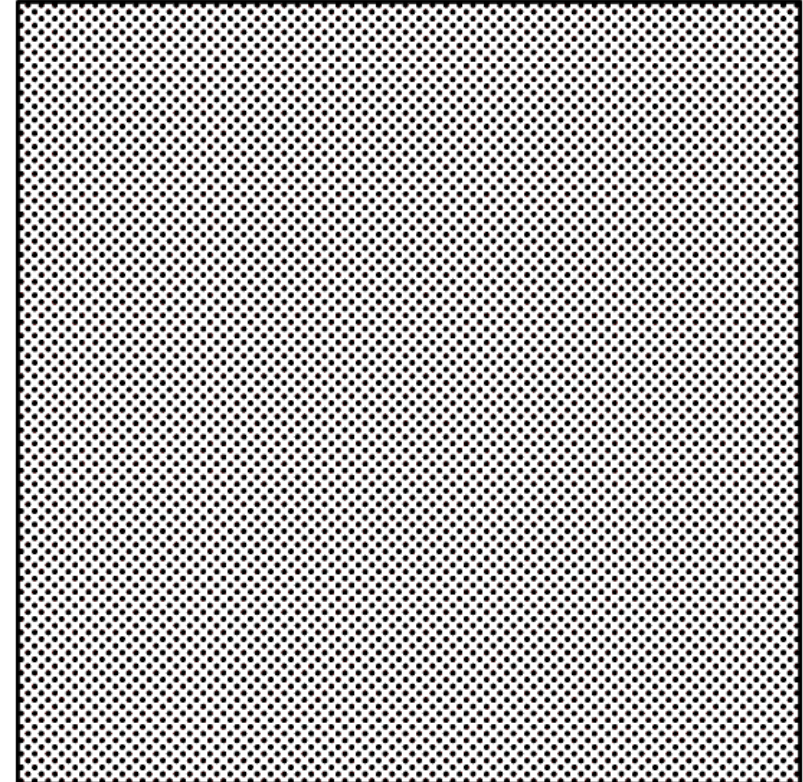
## From disorder to order





# Simulating primary radiation damage

- Give recoil to atom
- Evolve and watch the chaos
- Analyse produced defects
- But, requirements:
  - Robust interatomic potential
  - Efficient interatomic potential



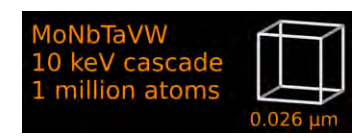
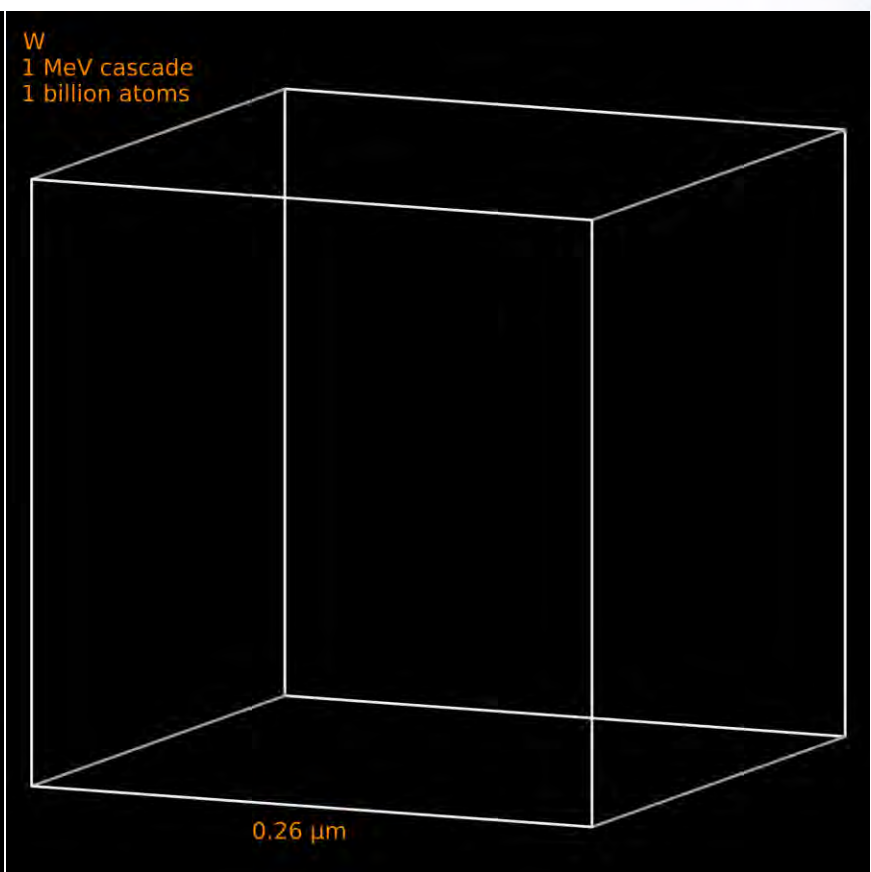
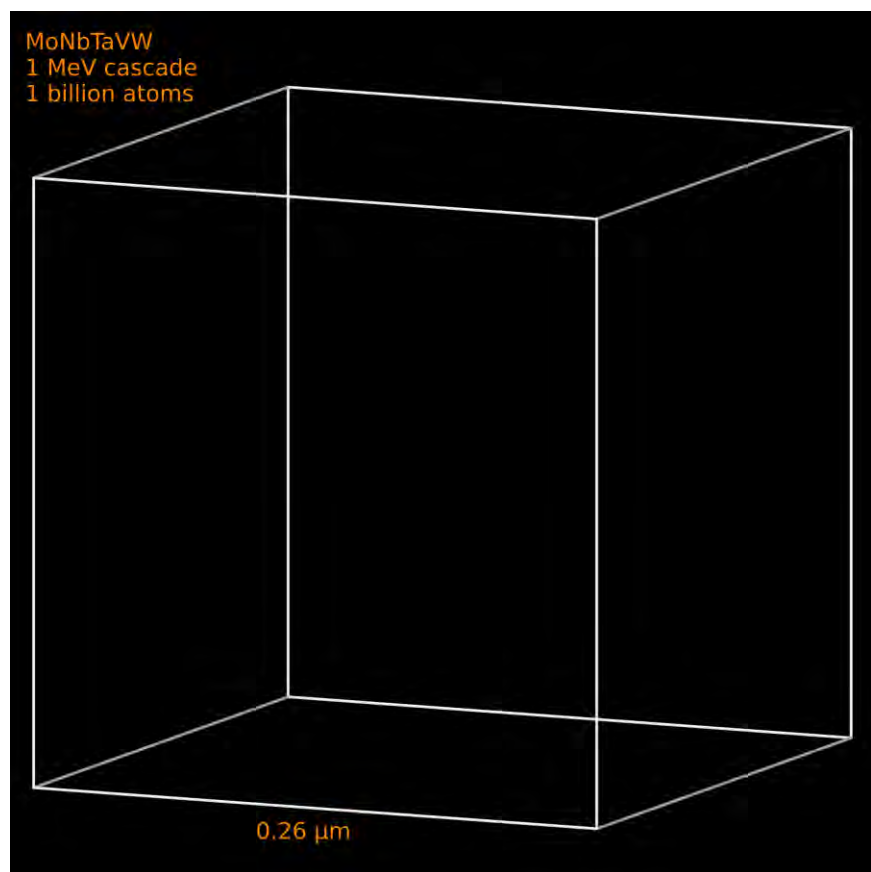


# Large-scale simulations of radiation damage



LUMI supercomputer in Kajaani  
• Fastest in Europe, 5th fastest worldwide

- GPU implementation and the LUMI cluster allow us to break records!
  - Ville-Markus Yli-Suutala (ÅA), Jan Westerholm (ÅA), Jan Åström (CSC), Aslak Fellman, Fredric Granberg (HU)





# Computational materials design: Searching for novel refractory alloys

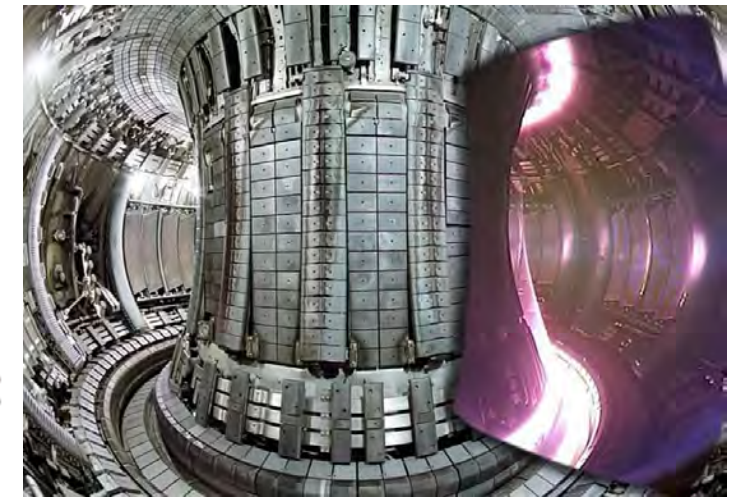
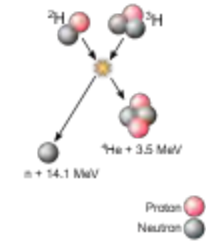
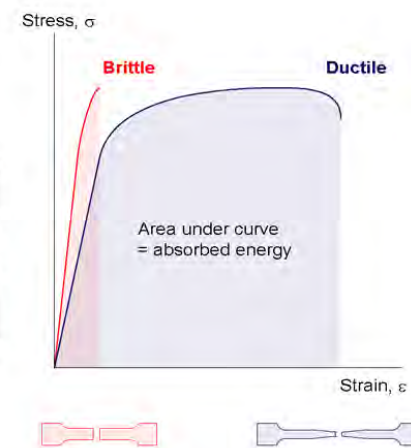
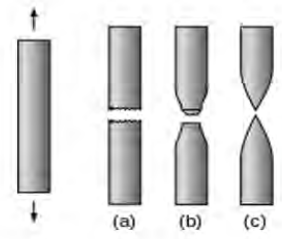
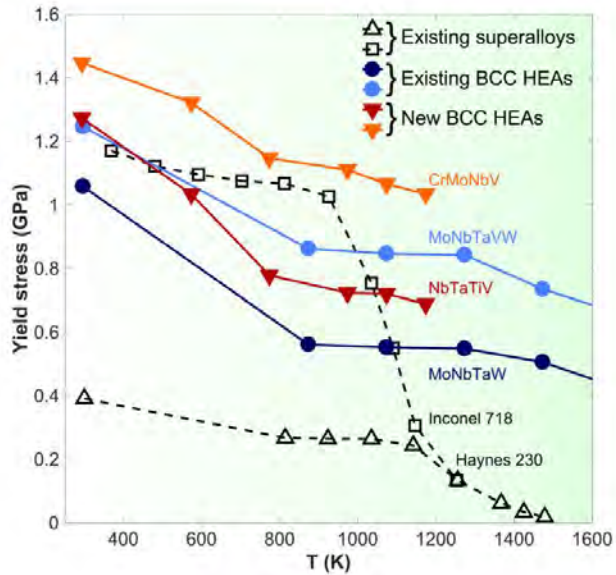
- The ideal alloy would be:
  - Strong
  - Ductile
  - Radiation-resistant
- Can we find promising compositions?
  - Refractory alloys (BCC crystal structure)



Periodic table of the elements

Alkali metals		Alkaline-earth metals		Transition metals		Other metals		Other nonmetals		Halogens		Noble gases		Rare-earth elements (21, 39, 57-71) and lanthanoid elements (57-71 only)		Actinoid elements				
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18			
1	H											He								
2	Li	Be											B	C	N	O	F	Ne		
3	Na	Mg											Al	Si	P	S	Cl	Ar		
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr		
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe		
6	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn		
7	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og		
lanthanoid series		6	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu				
actinoid series		7	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr				

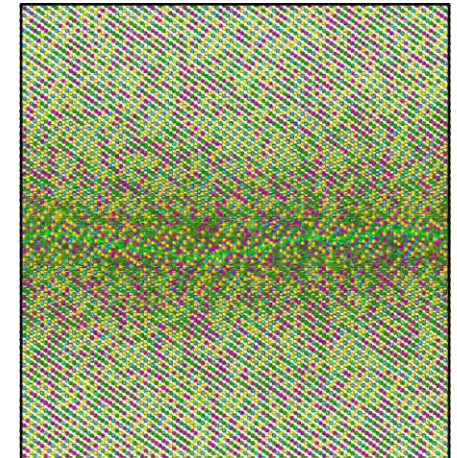
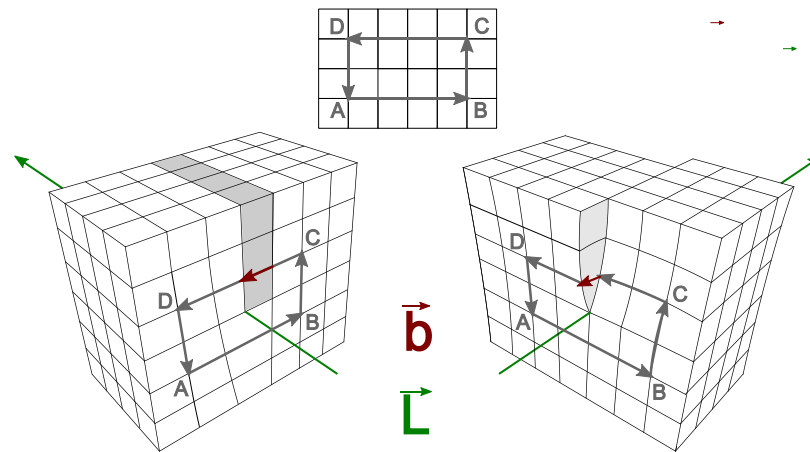
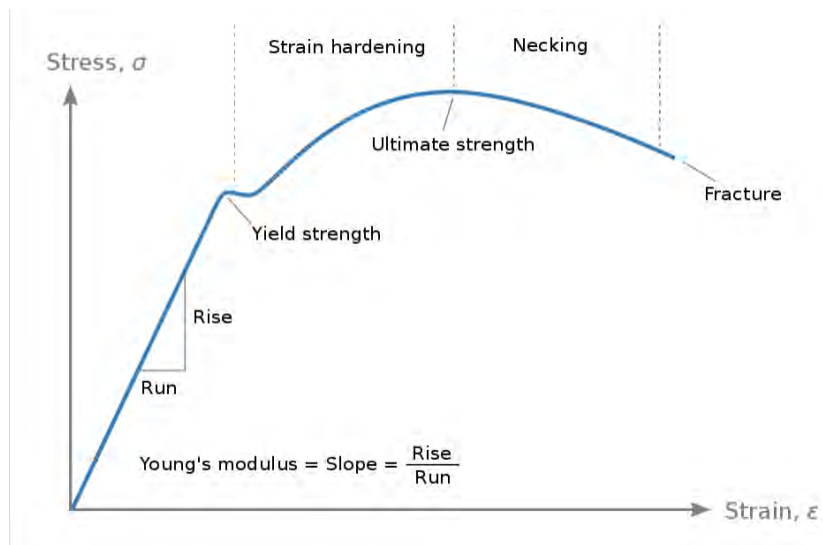
\*Numbering system adopted by the International Union of Pure and Applied Chemistry (IUPAC). © Encyclopædia Britannica, Inc.





# Simulating mechanical tests (strength)

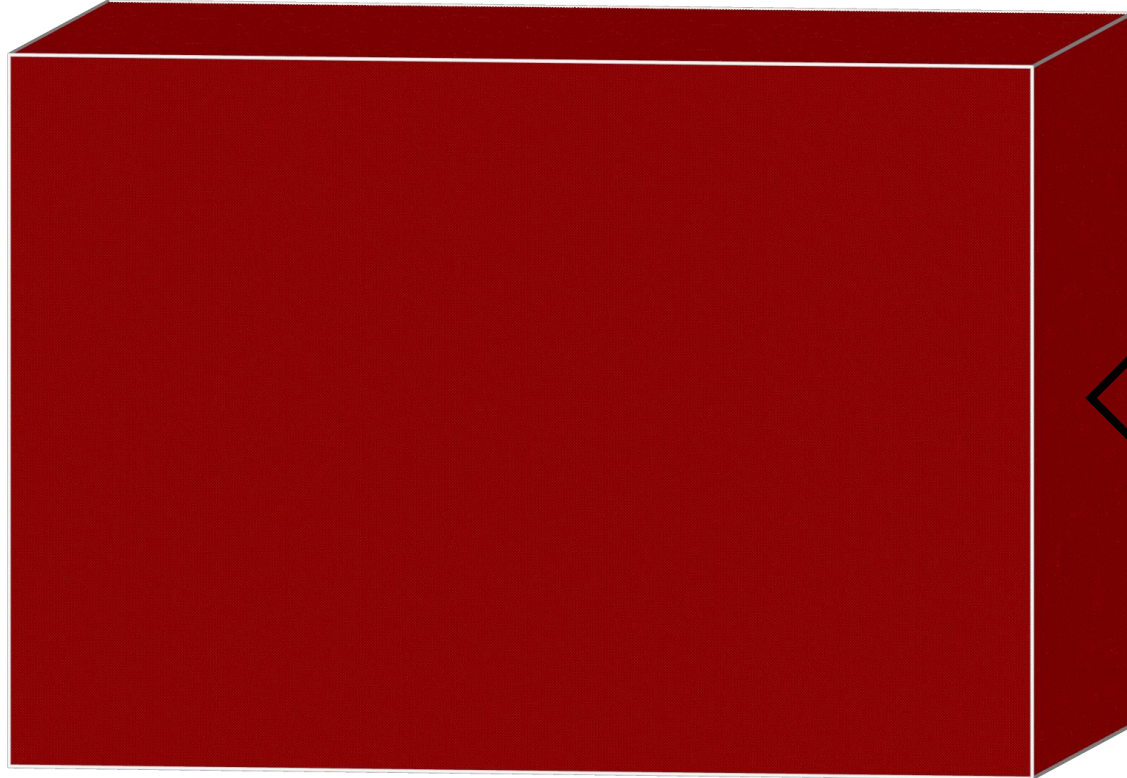
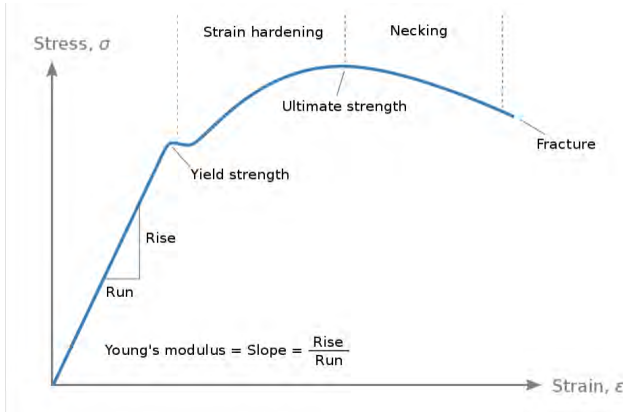
- What happens when we tear the alloys apart?
- Controlled by dislocations



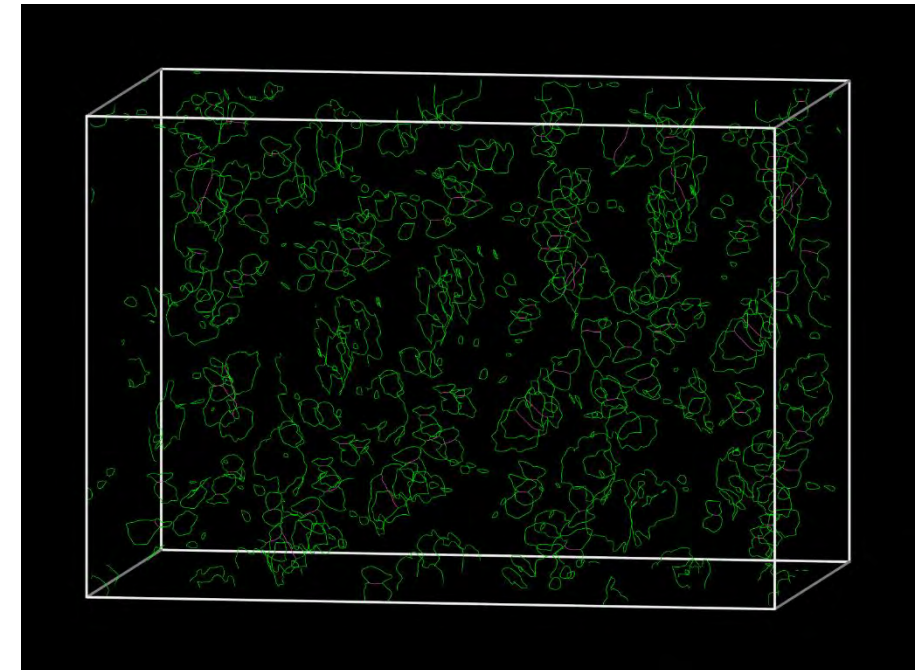
# Simulating mechanical tests (yield and plastic deformation)



- Pure W single crystal
- Irradiated
- 42.48 million atoms
- Compression rate  $5e7$  1/s

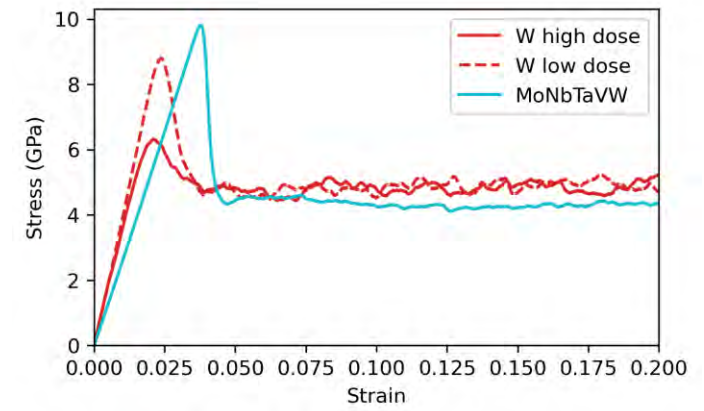


100 nm

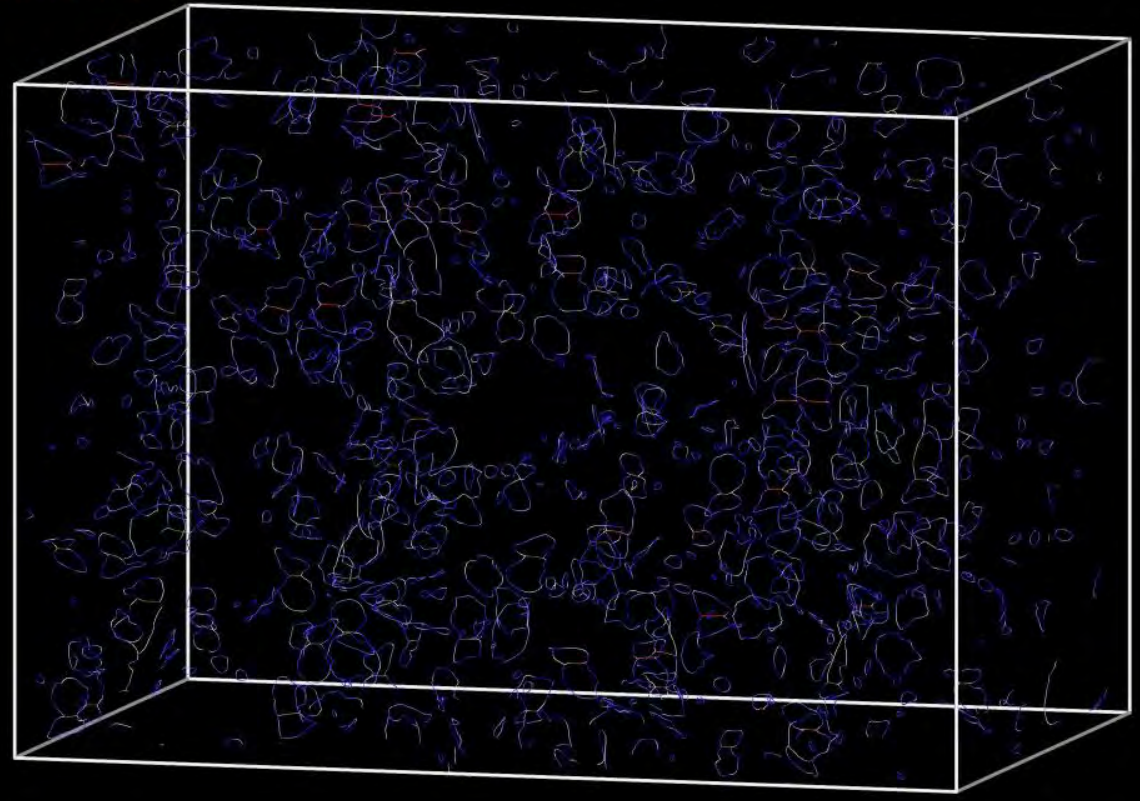




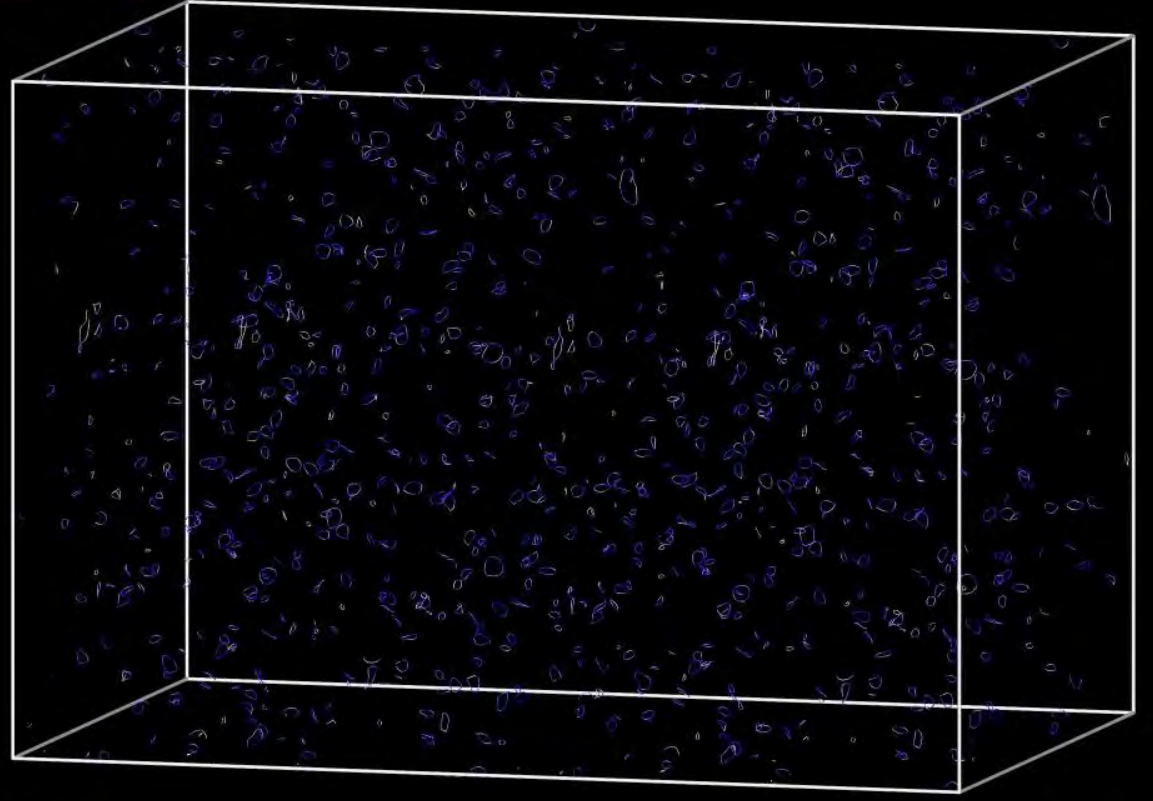
# Mechanical testing



W, Irradiated  
42.48 million atoms  
Compression,  $5e7$  1/s



MoNbTaVW, irradiated  
42.48 million atoms  
Compression,  $5e7$  1/s





# Conclusions

- Machine-learning interaction models (potentials) help us simulate complex materials and look for fusion-relevant alloys
- tabGAP: Fast, simple, accurate especially for alloys.
- Large-scale atomistic simulations of radiation damage, mechanical properties and plasticity.



Suomen Akatemia  
Finlands Akademi  
Research Council of Finland

**FCAI**

