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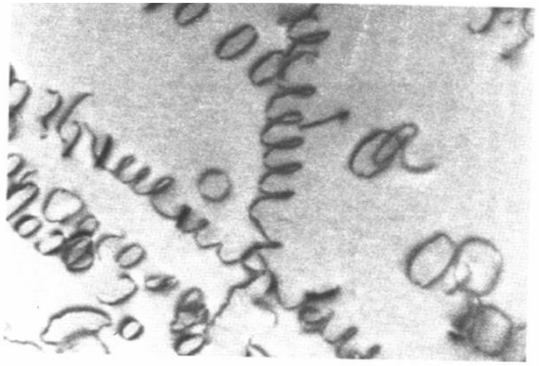
Radiation Damage Spring term 2014

9. Dislocation generation and evolution by irradiation

Dislocations

- **Dislocations** (*dislokationer / dislokaatiot*) are linelike defects in materials
- They exist in some finite concentration in all metals, and many other crystals as well, in equilibrium
- Mechanical processing and shape change of metals is usually all dominated by dislocations

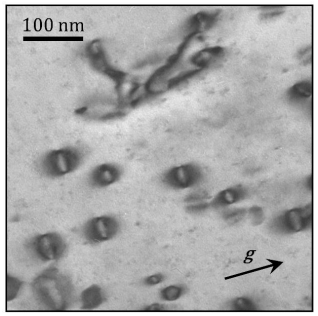


- Irradiation can often generate dislocations, and thus often modify the mechanical properties of materials

9.1. Dislocation generation by irradiation, part 1.

- Dislocations can be generated by irradiation in two (or two and a half) different ways

1. Dislocations can be generated directly in dense heat spikes
   - Either the vacancies or interstitial clusters, can, if large enough, directly collapse into a localized finite dislocation that starts and ends on itself, a **dislocation loop** (cf. previous chapter)

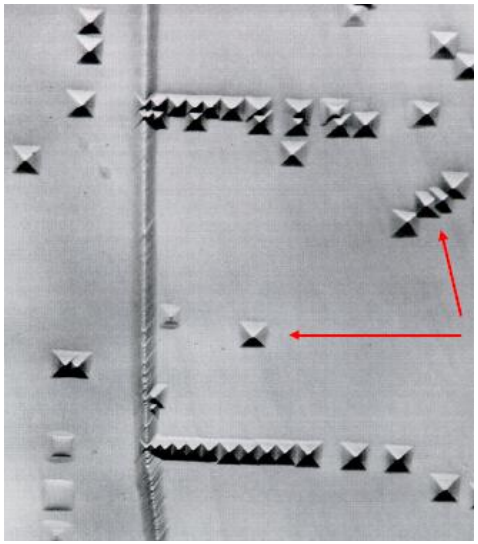


1.b. A vacancy or interstitial cluster can reform into a dislocation loop after the cascade is over

2. Atom migration can make point defects or small clusters later on coalesce into a dislocation loop

- Dislocations have for large sizes almost always a lower energy than a defect cluster, so thermodynamics tends to drive defects to form dislocations

9.2. Basics of dislocation properties



- Before continuing, we need to understand the basics of dislocations
- Dislocations are per definition linelike objects in a crystal
- The **dislocation core** (dislokationskärna / dislokaatioydin) is only a few atoms wide and hence from a macroscopic point of view can be considered dimensionless
- They can be made visible on a mesoscopic scale (in a light microscope) via chemical etching (etsning / etsaus), which etches more efficiently and thus enlarges the dislocation core
  - What becomes visible is a dislocation **etch pit** (*etsningsgrop / etsauskuoppa)* on the surface

Dislocations can be directly seen

- In a transmission electron microscope (TEM) dislocations can be observed directly, and even their mobility under suitable deformation or irradiation

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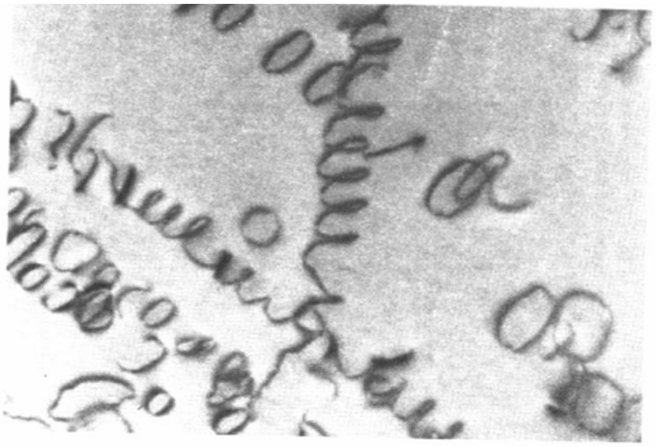
- Example to the right: dislocations formed in an Al-Mg alloy after rapid cooling

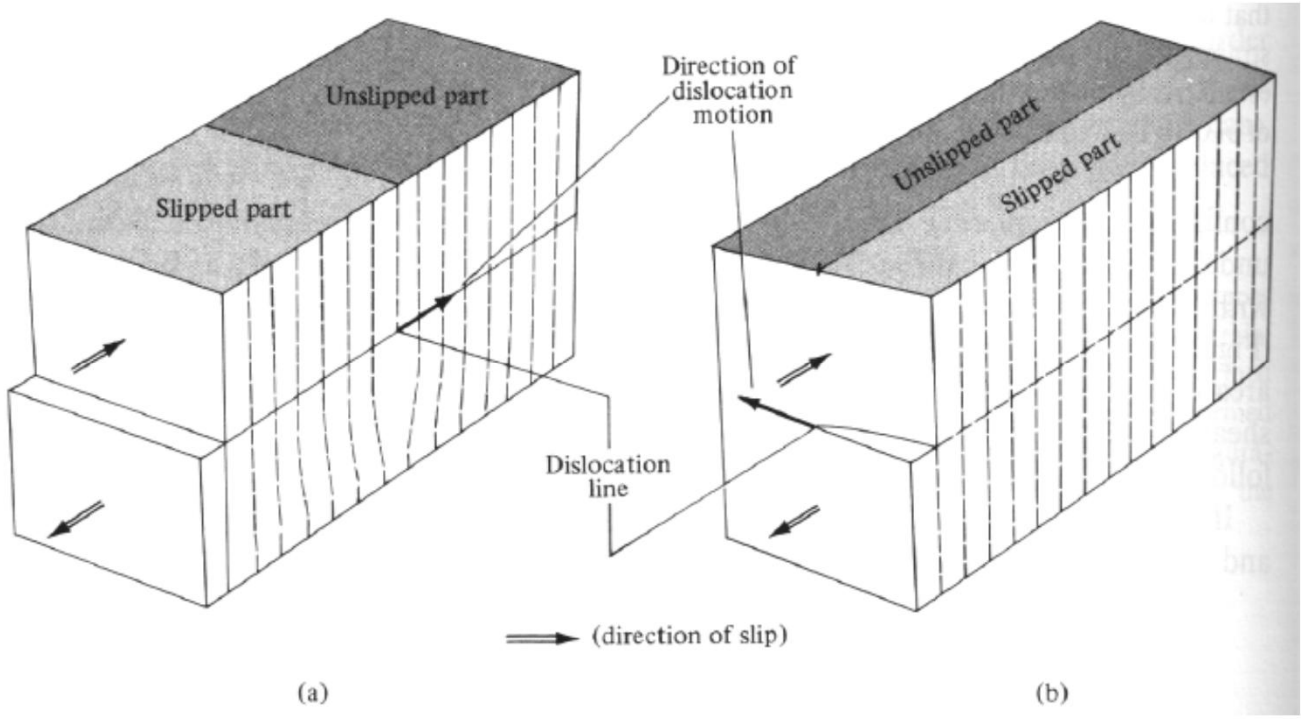


Two basic types of dislocations: edge and screw

- The formation of the two basic types of dislocations be understood in terms of the following two types of deformation of an imaginary crystal with crystal planes:

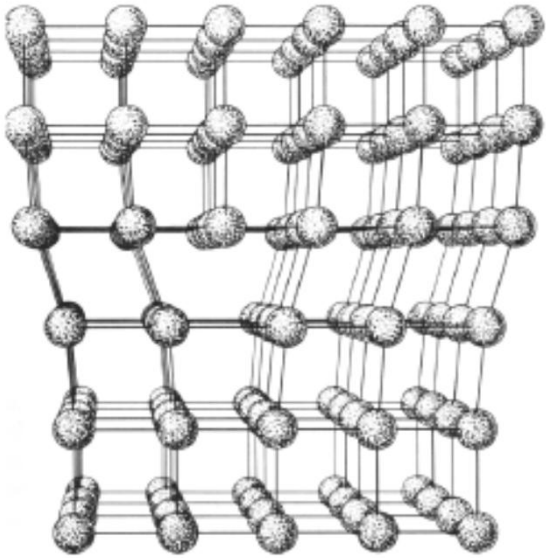
Edge dislocation (*kantdislocation / särmädislokaatio*)

Screw dislocation (*skruvdislocation / ruuvidislokaatio*)

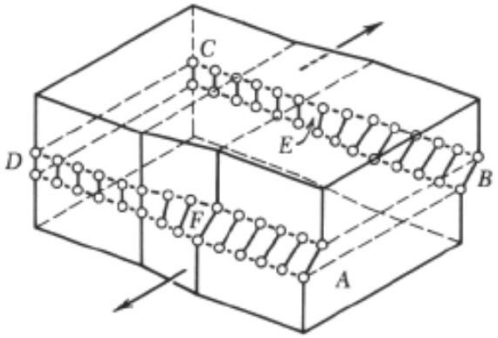


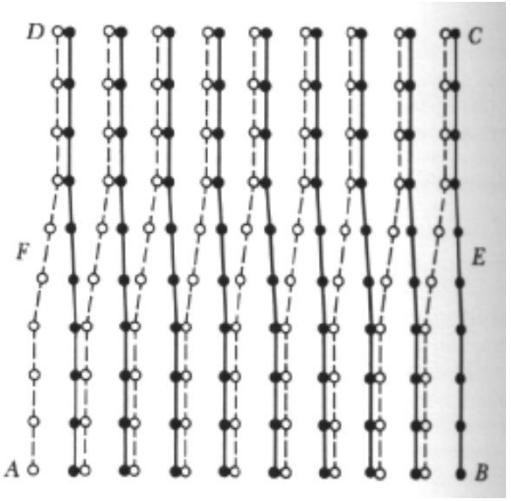
Atomic structure

- Atomic structure of an edge dislocation in a simple cubic lattice:



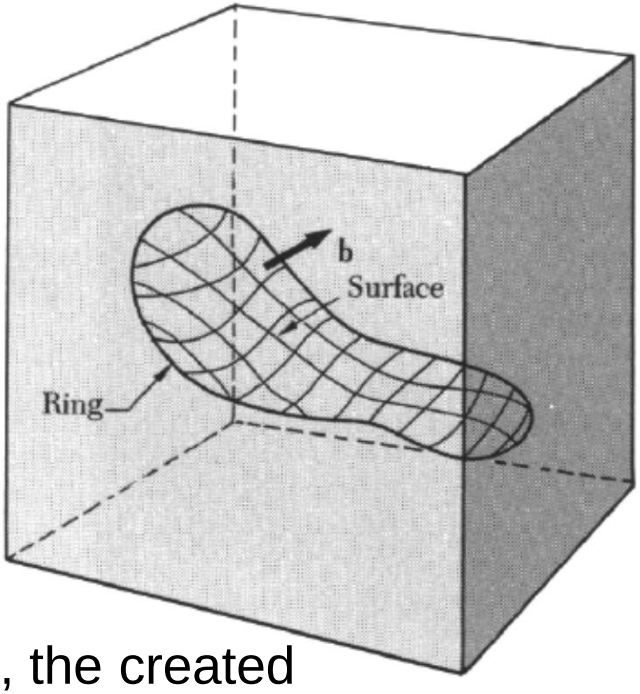
- Atomic structure of a screw dislocation:





General dislocations

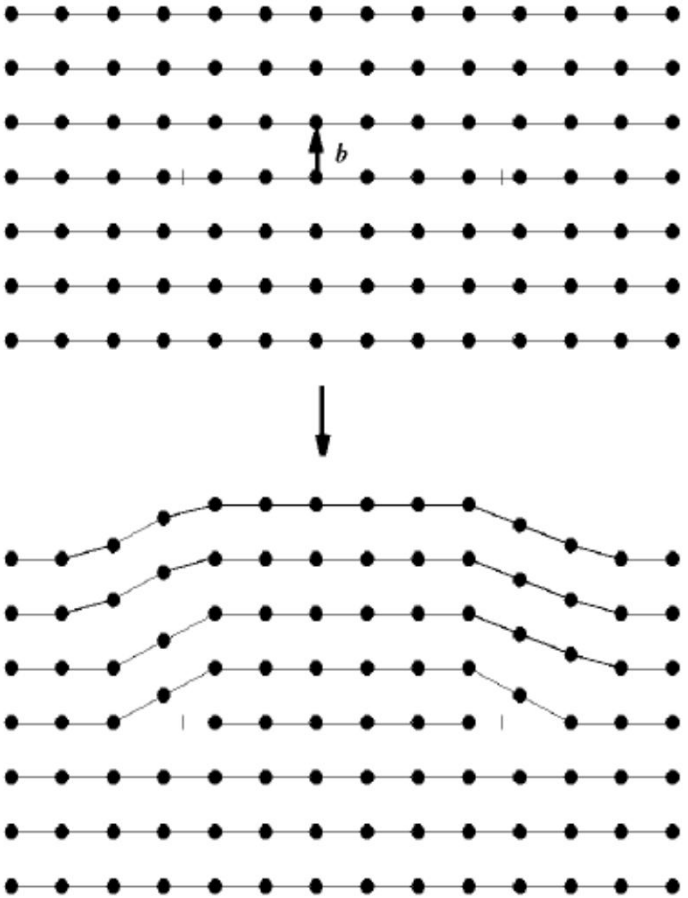
- In general a dislocation line segment does not need to be either edge or screw in character, but arbitrary in between
- The following *gedankenexperiment* explains how to form an arbitrary dislocation:
  - Select an arbitrary surface inside a crystal.
  - Remove the material on one side of the crystal, and move it by a displacement vector **b** . Fill then in the void that was created with new atoms, or if **b** is negative, take away the material



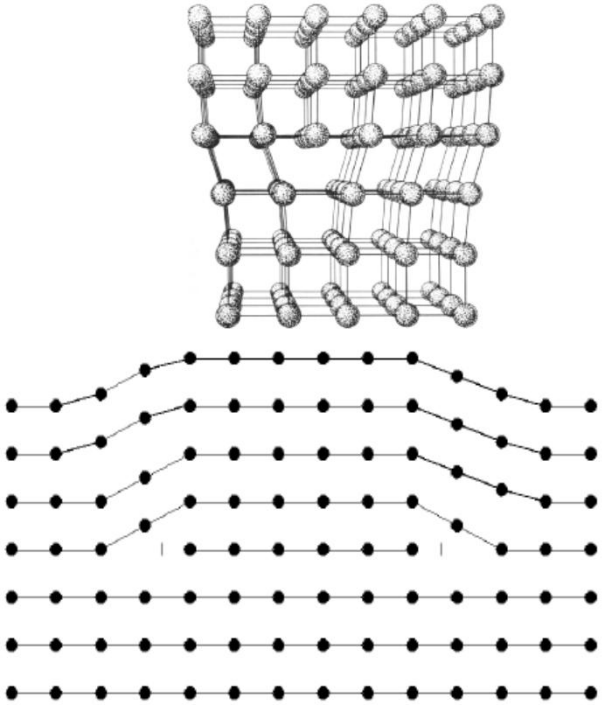
- If **b** is chosen such that the atoms that fill in the surface form again perfect crystal, the created dislocation is called **a perfect dislocation**. Otherwise it is a **partial dislocation** (partiell dislokation / osittainen dislokaatio)

Burger's vector

- A simple example of this in a quadratic lattice is illustrated here
  - The vector **b** is the ***Burger's vector***.
  - Note that the crystal far away from the dislocation core is practically perfect
  - But there is always a weak strain field that weakens but in principle extends to infinity



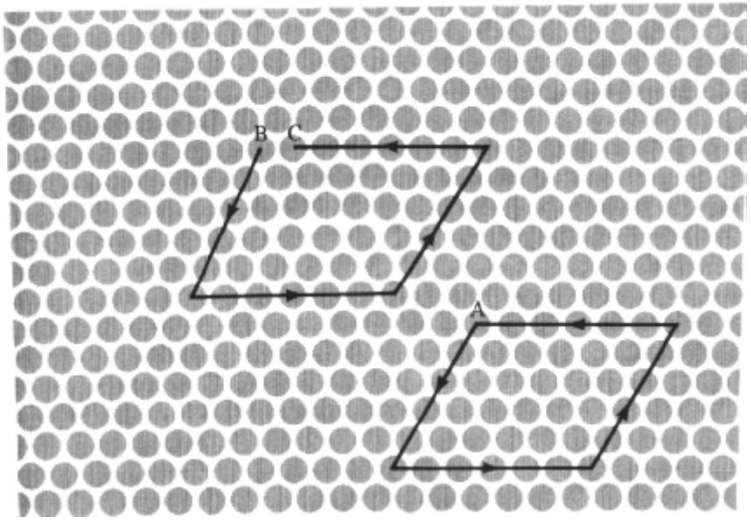
Character of (edge) dislocations



- For a general dislocation that ends at a surface, it is a matter of definition whether one says that one row of atom was added or another was removed
- But for dislocation loops inside a crystal, one can make a distinction between atom addition and removal
- If atoms have been added, one can talk about an ***extrinsic dislocation*** or ***interstitial-type dislokation***
- If atoms have beeb removed, one talks about an ***intrinsic dislocation*** or ***vacancy type dislokation***

Deriving the Burger's vector

- For a general perfect dislocation, the following operation can be used to deduce its Burger's vector
  - First consider a perfect region of a crystal. Draw vectors that follow the nearest-neighbour interatomic distances such that they form a closed loop
  - Then repeat the same number of steps around the dislocation. Now the loop will not be closed, and the vector needed to close it is **b** (its sign is arbitrary).



- If **b = 0** it is not per definition a dislocation
- Note that there are line defects that are not dislocations: e.g. a long row of vacancies is a line defect but not a dislocation!

Stacking faults

- An important type of two-dimensional defects are **stacking faults** (*radningsfel / pinovirheet*).
- The standard example are those in FCC metals
- Recall from the crystal structure courses that an FCC crystal is formed by putting close-packed 2D hexagonal planes above each other (stacking them) as

  ABCABCABC...

  whereas a HCP crystal is formed by putting the same layers in the order

  ABABABAB....

Stacking faults

- For hard spheres, the energy of the two crystals would be identical. Hence it is easy to understand that changing the stacking sequence such that the atom are still above the wholes in the next layer would not make a big difference in energy => easy to form a defect
- For instance in the FCC-lattice one can change

  ABCABCABC to ABCAB**A**CABC

- This extra plane can extend all the way to the surface, but if it ends insid the crystal, it can considered to be a planar (2D) defect surrounded by partial dislocations!
- Turns out stacking faults are easy to form especially in FCC crystals and hence partial dislocations are also common in them

Stacking faults

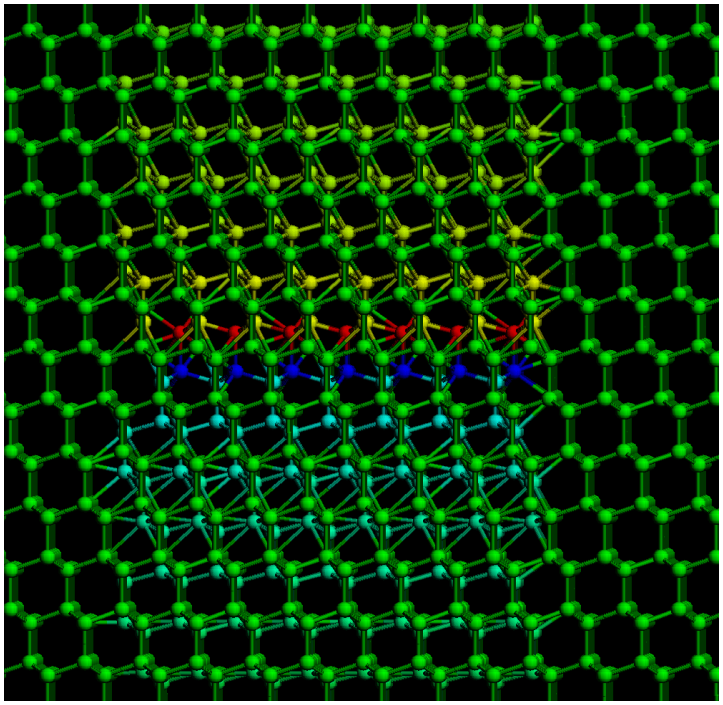
- Because the diamond crystal structure can be considered to be two interpenetrating FCC lattices, the same operation can also be done in the, but one needs to consider double planes to preserve the 4-fold bonding of all atoms:

  AaBbCcAaBbCcAaBbCc

  to

  AaBbCcAaBb**Aa**CcAaBbCc

- This defect is illustrated to the right with the red and blue atoms being the extra ones



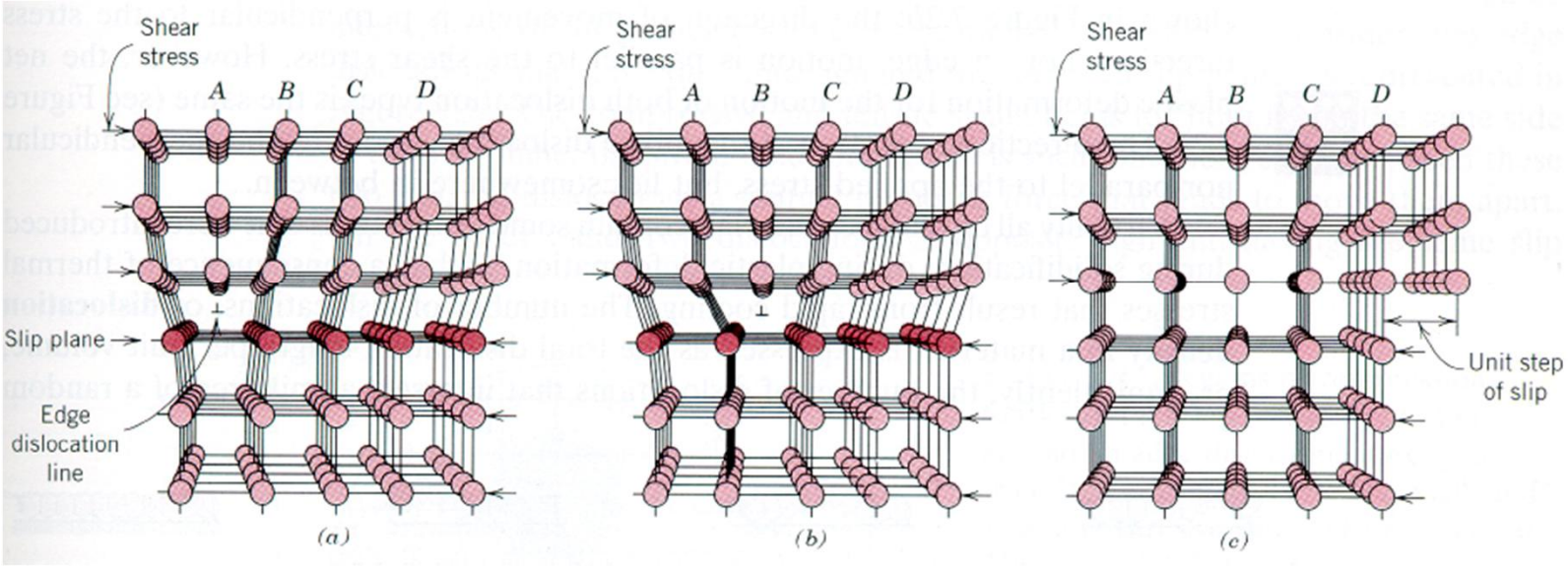
[K. Nordlund et al, Appl. Phys. Lett. 76 (2000) 846]

Dislocation densities without and with irradiation

- The amount of dislocations can be given as number/area
- Typical dislocation densities [Callister]:
  - Well-crystallized metals : ~ 10^3 1/mm^2
  - Heavily deformed metals: ~ 10^9 - 10^{10} 1/mm^2
- Irradiation generally generates dislocation loops, and they can obtain extremely high densities
  - Upper limit estimate: assume one heat spike has a spherical shape with a radius = 3 nm. If one dislocation loop is generated in this, and one intersects it on two points, the local density then becomes $2/(\pi\ 3\ \text{nm})^2 \approx 0.1$ 1/nm^2 = 10^{11} 1/mm^2
  - On prolonged irradiatio, this could also become the global dislocation density – unless they migrate and grow

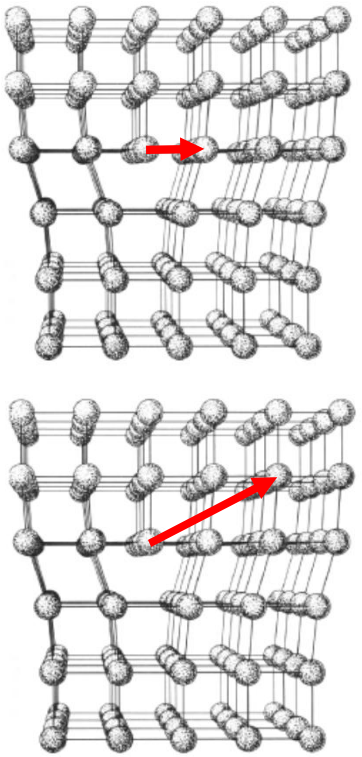
Dislocation mobility

- The reason dislocations are associated with plasticity of materials is that they are often very easily mobile
- No atom moves a lot, but a dislocation can move macroscopic distances
- Easily mobile dislocations are called **glissile**, the others **sessile**



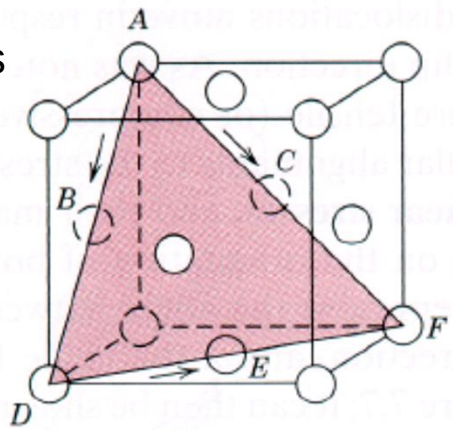
Dislocation mobility

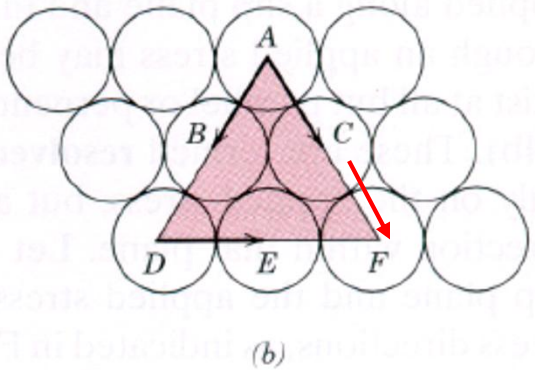
- The dislocation mobility can easily only occur in certain well-defined crystal directions
- This is easy to understand intuitively, looking at e.g. the pictures to the right



Glide systems

- The crystallographically favourable directions for dislocation motion are called the **glide** or **slip directions (***glidriktning* / liukusuunta) and the plane along which it occurs the **glide** or **slip plane** (*glidplanet / liukutaso**)***
- The combination of the two is called the ***glide system (****glidsystem / liukujärjestelmä)*
- Considering the FCC crystal, built up of the hexagonal close-packed 2D planes lying on 111 planes, it is pretty easy to understand that glide of an edge dislocation can occur easily perpendicular to the 111 plane . To get from one atom position to another sensible position, the atom motion must be in the 110 direction
- But to form stacking faults or partial dislocation, the movement can be another, $11\bar{2}$





Glide system

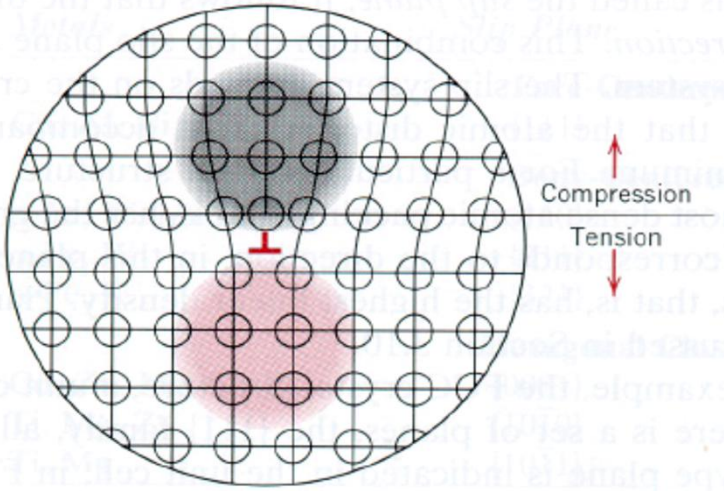
- In other crystals it is not equally obvious what the glide system would be, but here is a list of the most common observed ones in metals [Callister]:

Table 7.1 Slip Systems for Face-Centered Cubic, Body-Centered Cubic, and Hexagonal Close-Packed Metals

Metals	*Slip Plane*	*Slip Direction*	*Number of Slip Systems*
	Face-Centered Cubic		
Cu, Al, Ni, Ag, Au	{111}	$\langle 1\bar{1}0 \rangle$	12
	Body-Centered Cubic		
α-Fe, W, Mo	{110}	$\langle \bar{1}11 \rangle$	12
α-Fe, W	{211}	$\langle \bar{1}11 \rangle$	12
α-Fe, K	{321}	$\langle \bar{1}11 \rangle$	24
	Hexagonal Close-Packed		
Cd, Zn, Mg, Ti, Be	{0001}	$\langle 11\bar{2}0 \rangle$	3
Ti, Mg, Zr	$\{10\bar{1}0\}$	$\langle 11\bar{2}0 \rangle$	3
Ti, Mg	$\{10\bar{1}1\}$	$\langle 11\bar{2}0 \rangle$	6

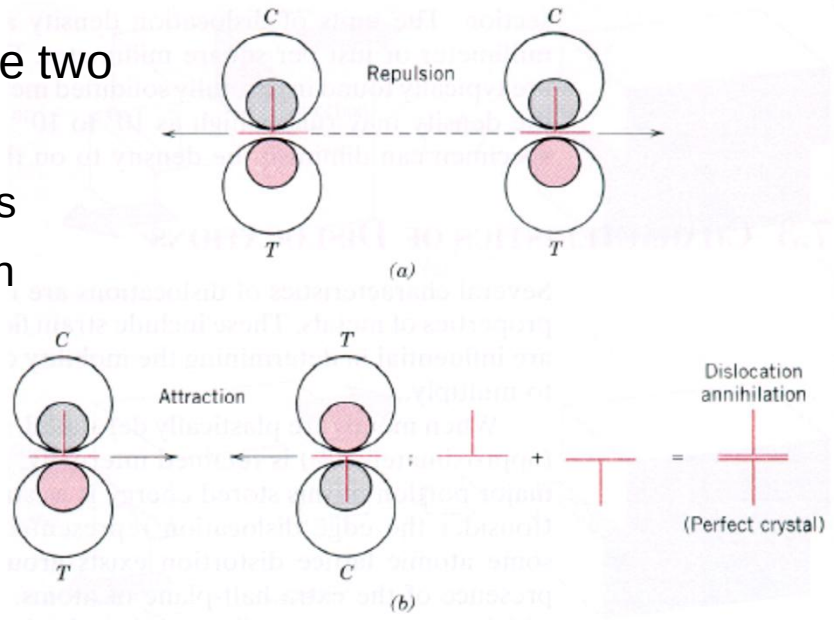
Dislocation reactions

- Dislocations can also interact and react with each other
- Each dislocation is surrounded by a strain field, and these enable a long-range interaction
- For edge dislocations it is of the following type: positive (compressive) on one side, negative (tensile) on the other
- The field is thus analogous to that of a dipole, although the functional form is not the same



Dislocation reactions and DDD

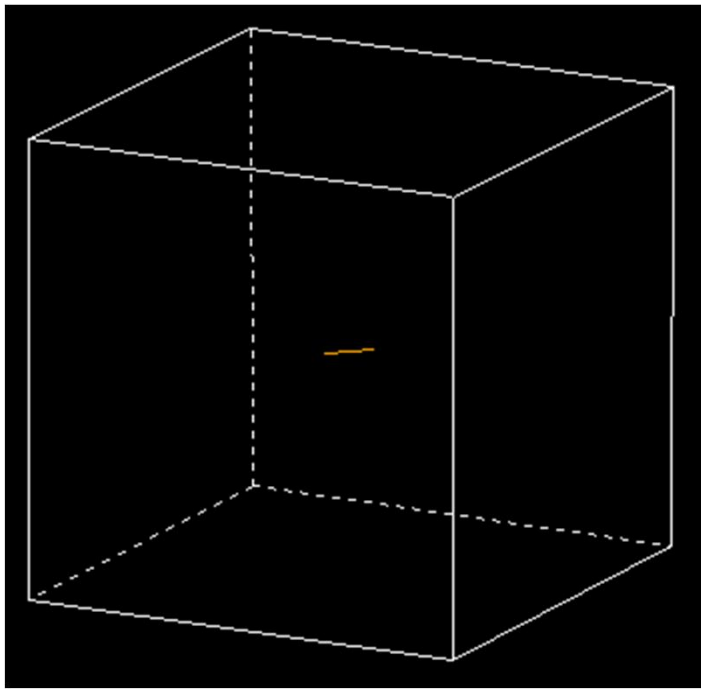
- The adjacent picture illustrates the two simplest possible interactions:
  - (a) two identical edge dislocations oriented the same way repel each other
  - (b) two identical but opposite-oriented dislocations attract each other and can annihilate perfectly(!)



- Due to these strain field interaction, dislocation can be modelled as a set of interacting line segments
- There is a simulation technique that uses these interactions and the a molecular-dynamics-like algorithm to solve the motion of dislocations, ”**discrete dislocation dynamics** (DDD)”

Dislocation creation

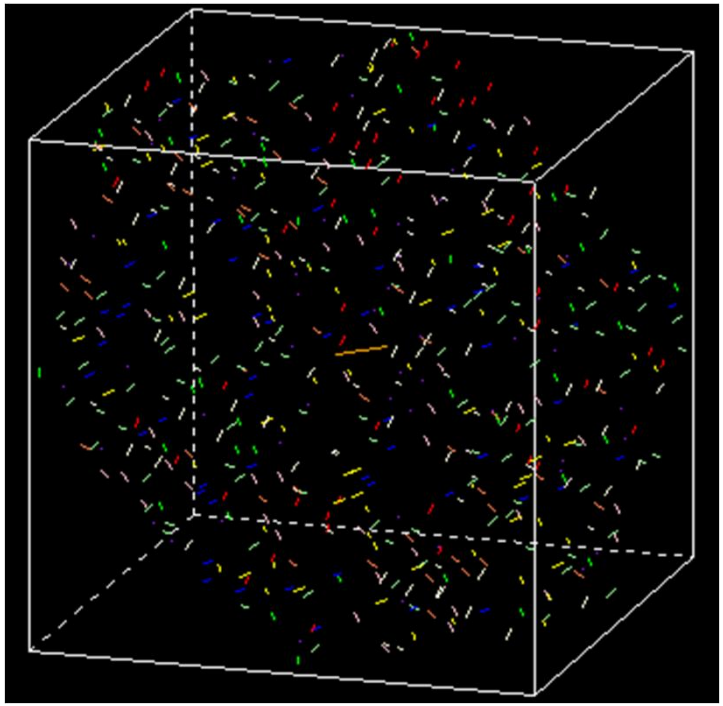
- Dislocations can also be created and annihilated by dislocation sources
- One important example is the ***Frank-Read-source***, which Is formed by two dislocation obstacles with a dislocation in betweem



- If now a pressure is set on the crystal, the dislocation can grown and multiply, see attached DDD-animation
- This process can repeat itself

Dislocation obstacles

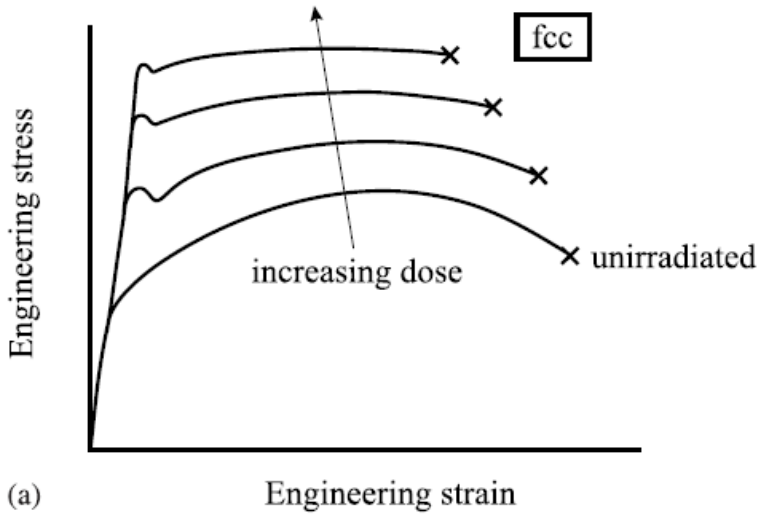
- The motion of one dislocation can be slowed down by others
- This is illustrated in the attached animation of a Frank-Read source in the middle, surrounded by small dislocation segments
- Animation shows how they slow down the movement

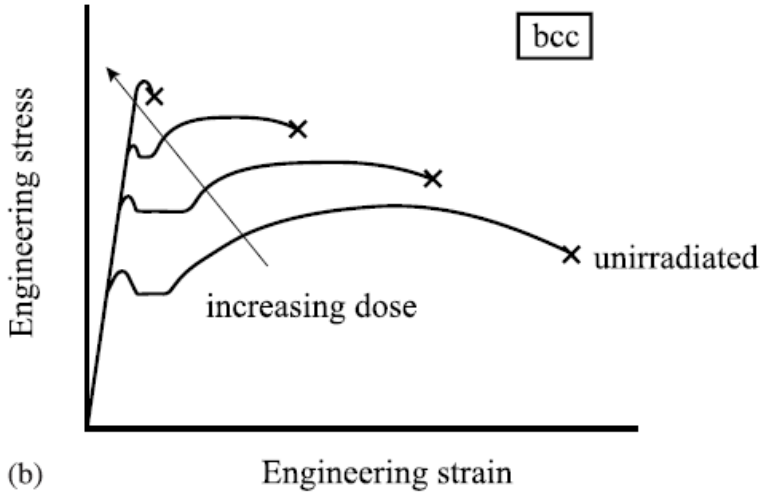


- The dislocation loops and other defects created by irradiation can have exactly this effect!

Effect of irradiation on mechanical properties

- Slowing down of dislocation motion in metals generally makes the material harder and more brittle
- Thus irradiation can (by creating dislocation obstacles) make metals harder and brittler
- Illustration from [Was] book for fcc (austenitic) and bcc (ferritic) steels



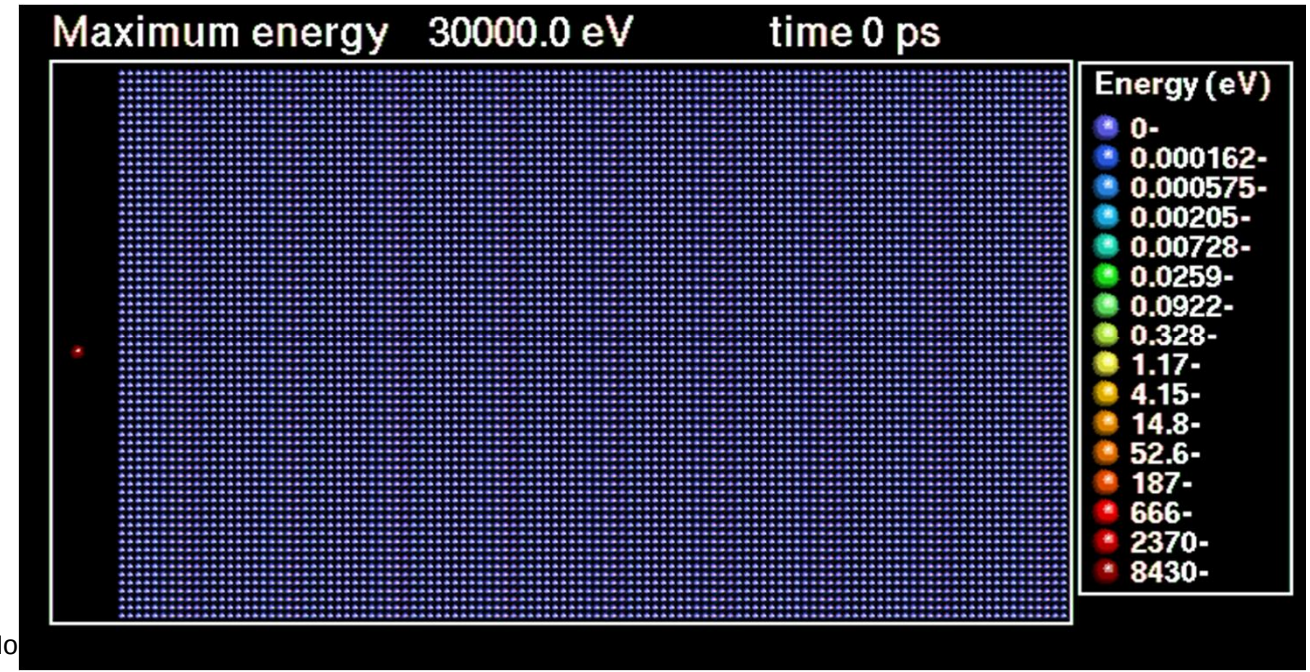


Annealing

- The dislocation created by material deformation or irradiation can often at least partly be removed by annealing. Simply by heating up the material, one can get back some or all of the original properties. This is called **annealing** (*glödgning / hehkutus*)
- Annealing can be further subdivided into **recovery** (*återhämtning / palautuminen*)**, recrystallization** (*rekristallisation / uudelleenkiteytyminen*) and ***grain growth*** (*korntillväxt / kidekasvu*)
- The first stage means defect removal, the latter ones involve changes of the overall microstructure of the material

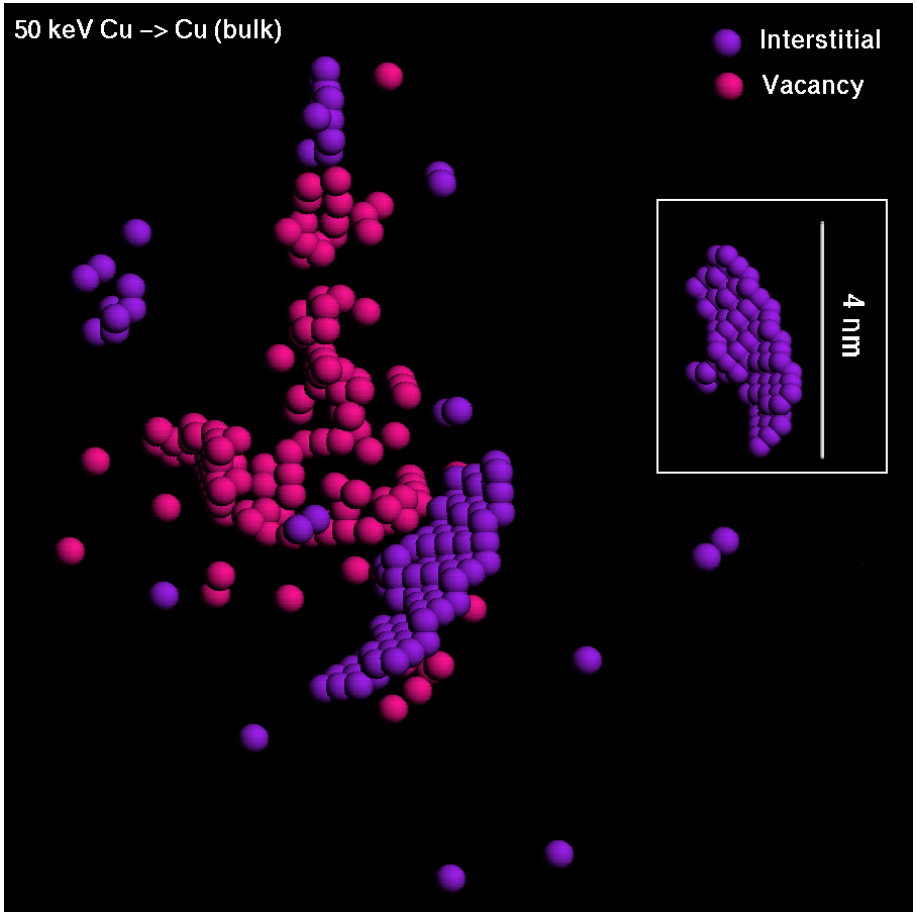
9.3. Dislocation generation by irradiation, part 2

- Now that we understand the basic dislocation properties, it is easier to present their formation
- Consider the old movie:
- The line-like features formed to the right are clearly parts of dislocations



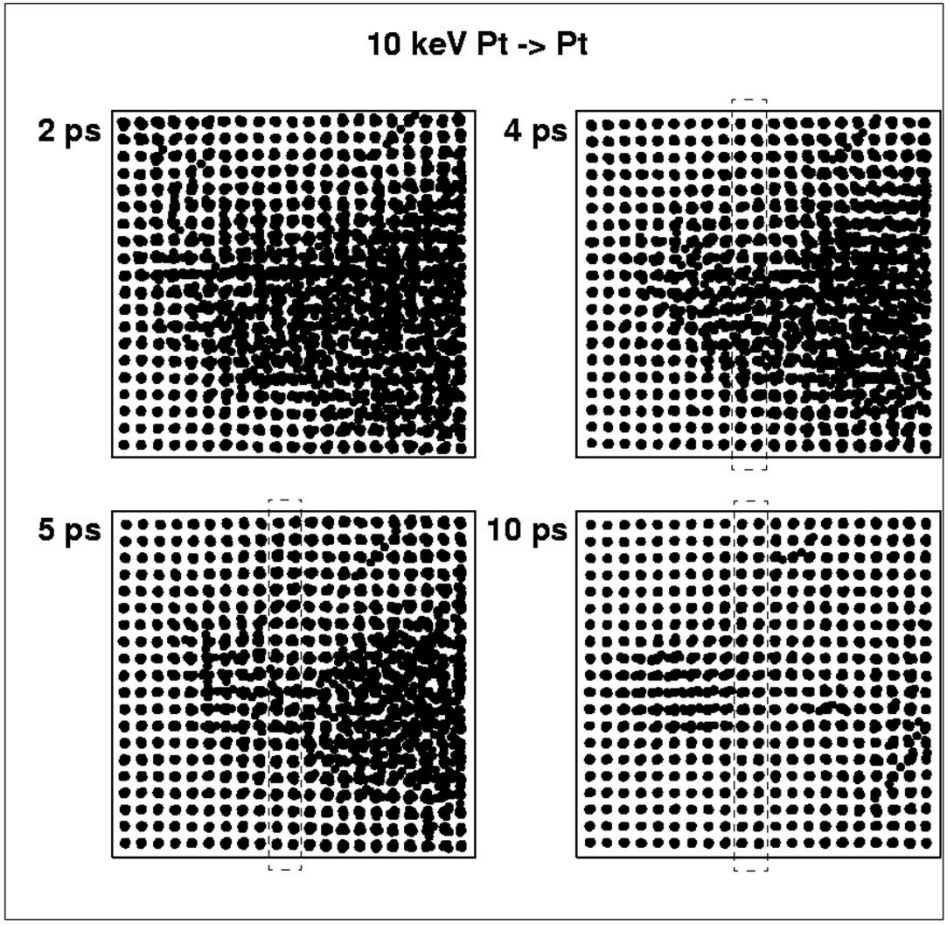
Interstitial loop generation

- By analyzing for the interstitial and vacancy atom positions and plotting only these, one can better understand whether the defects are really dislocations
- Heat spikes can sometimes indeed form directly fairly well-ordered interstitial dislocation loops



Liquid isolation mechanism

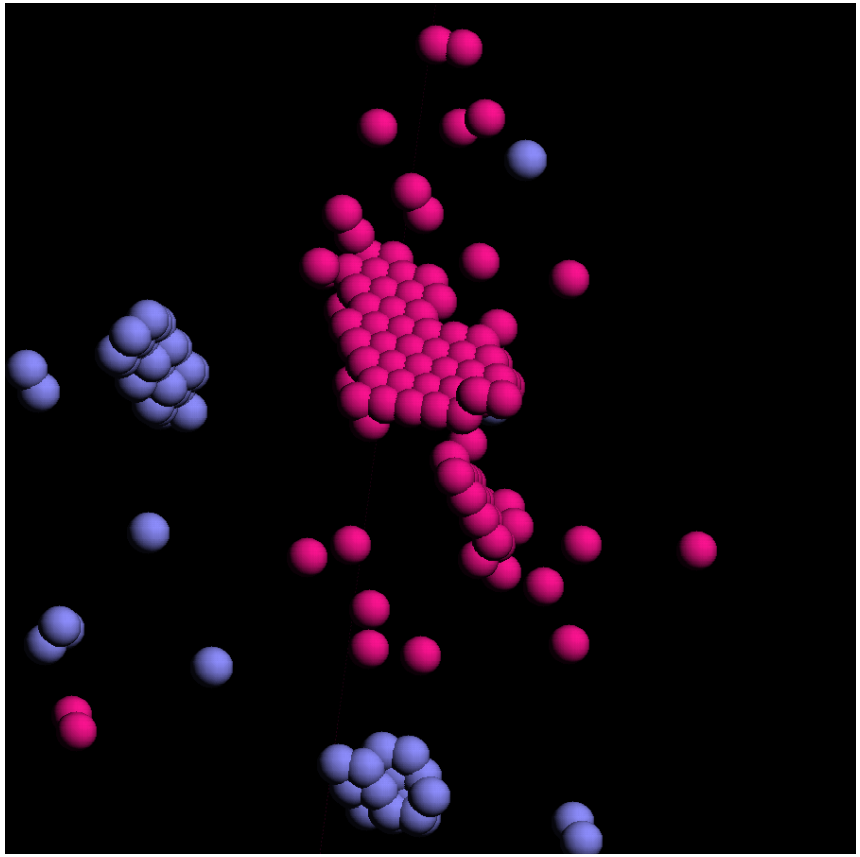
- Detailed analysis showed that such ordered interstitial clusters can be produced due to recrystallization
  - "Liquid isolation mechanism"'
- The groups of (at least) Roger Stoller and David Bacon have analyzed a big number of interstitial clusters produced in cascades and determined their dislocation character



[Nordlund et al, PRB 57 (1998) 7556]

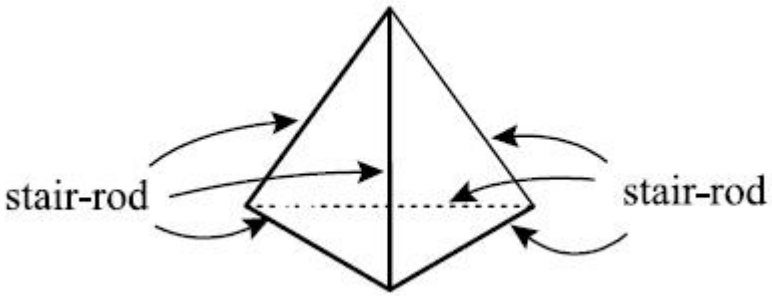
Vacancy cluster formation

- The vacancy clusters typically are disordered, but already directly close to the shape of an dislocation loop
  - With some annealing (even room temperature enough) it is quite likely these become well-ordered dislocation loops

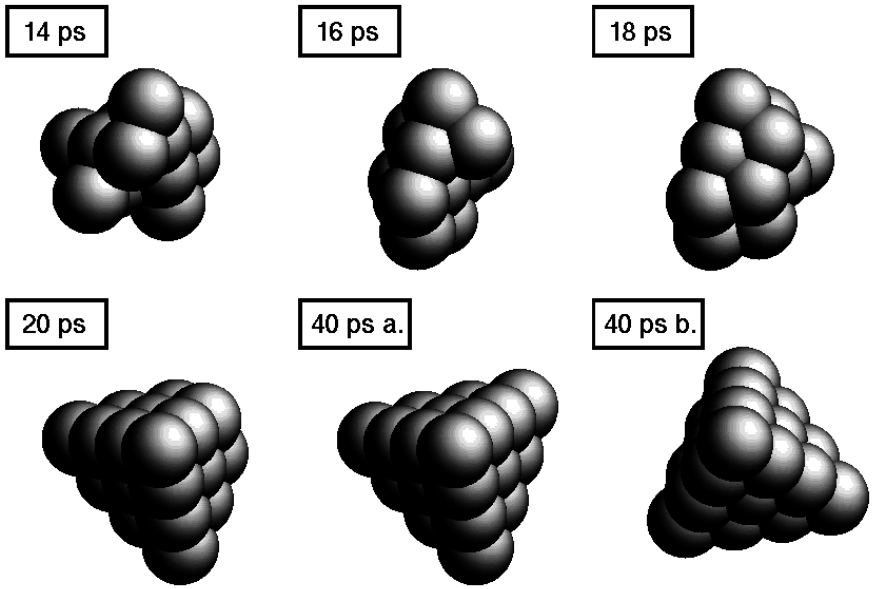


Stacking fault tetrahedra

- Several experiments have shown that a special kind of tetrahedral pyramid, a **stacking fault tetrahedron** (SFT), can form in FCC metals like Cu already at 20 K
  - This is 4 stacking fault triangles forming a pyramid bound by partial, so called stair-rod, dislocations
- MD simulations showed that these can indeed directly form in a single collision cascade



[Was]

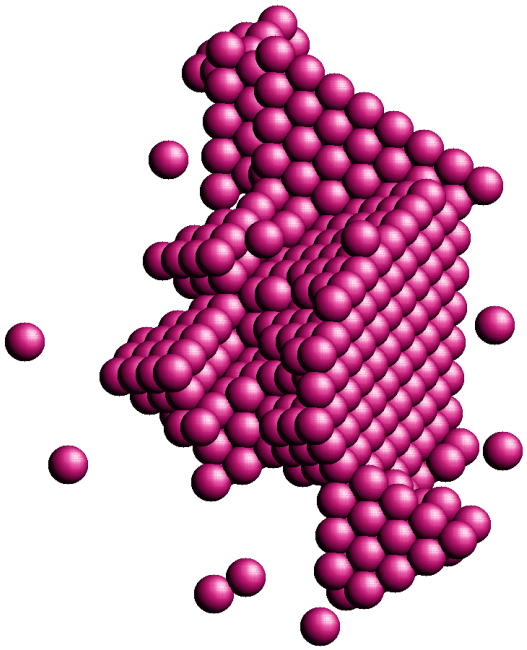


[Nordlund and Gao, APL 74 (1999) 2720]

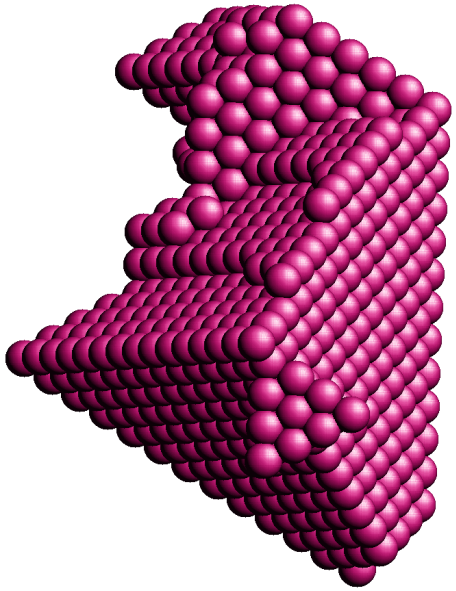
Reshaping to form an SFT

- Even bigger ones can form after moderate times for allowing reshaping of vacancies into a lower-energy state

Initial cluster shape from MD cascade



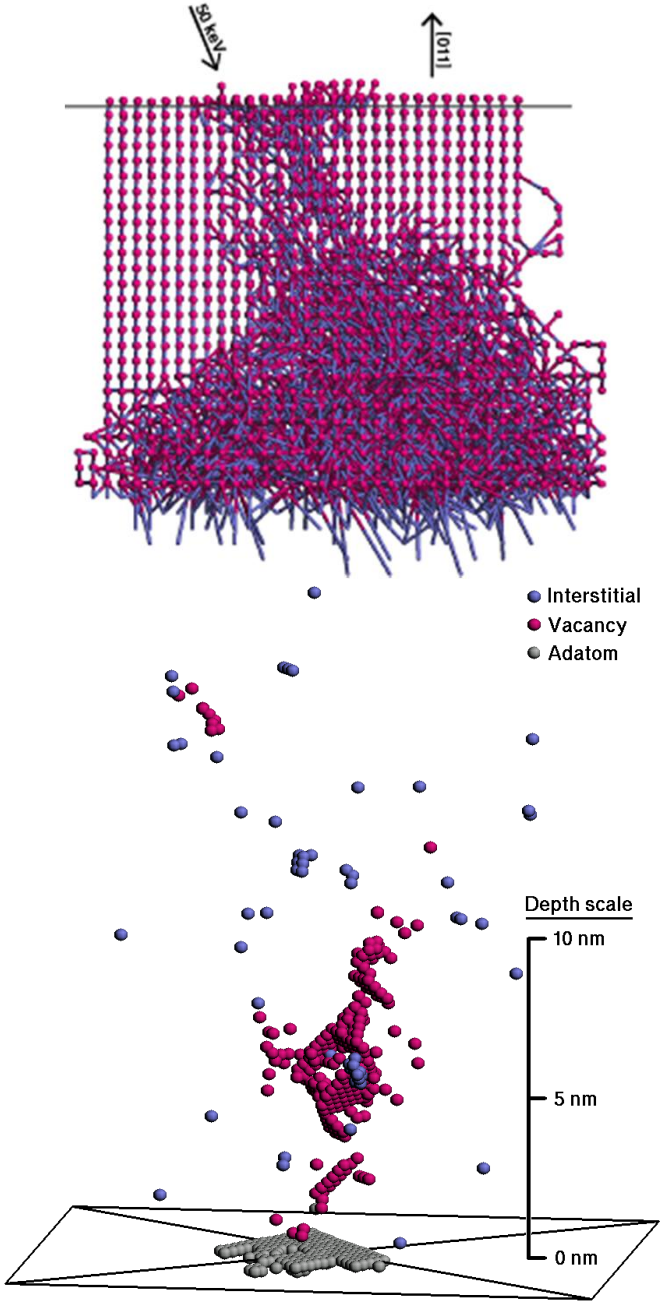
After 1 ns at 800 K



[Nordlund and Gao, APL 74 (1999) 2720]

Surface effects

- Near surfaces, the defect generation can be enhanced in a major way due to atom flow to the surface
- This can be considered to be **dislocation loop punching** to the surface, i.e. creating an interstitial loop in the cascade that glides to the surface along the dislocation 110 glide direction



[Nordlund et al, Nature 398 (1999) 6722]

9.4. Dislocation mobility and its slow-down

- As stated above, dislocations can move easily
- In MD simulations, it appears that the dislocation motion activation energy is for some common types of dislocations of the order of 0.01 eV, i.e. extremely low!
- But recent experiments indicate higher activation energies, e.g. about 1 eV for 111 loops in Fe [Arakawa, Science 318 (2007) 956]
- The reason to the discrepancy seems to be that dislocations bind to impurities like C and O (which are always present in metals) with activation energies around 1 eV, and hence the inherent ’pure’ dislocation mobility of 0.01 eV cannot be observed – but this is not yet fully certain

Dislocation mobility slow-down: Cr in Fe

- Also alloying elements can slow down dislocations
- For instance, recent work on stainless steels, which per definiction contain ~10% Cr, indicates that the mobility of the dislocations is slowed down by the Cr atoms when compared to pure Fe

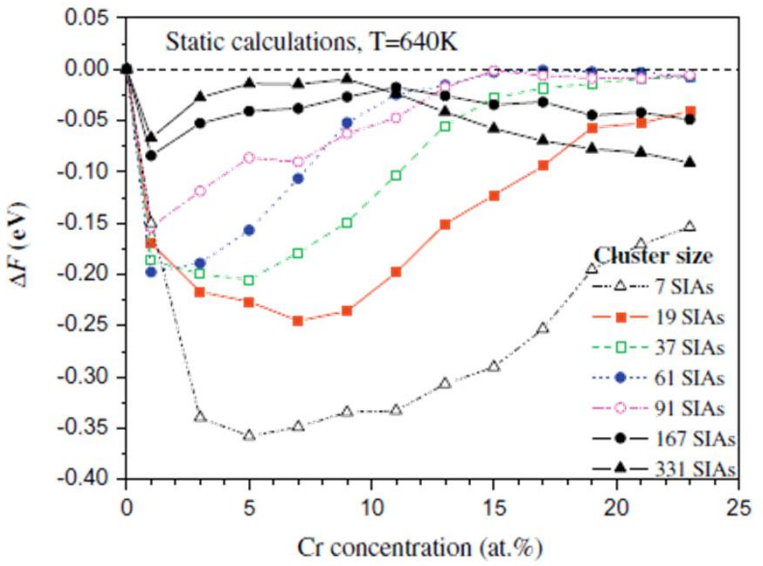
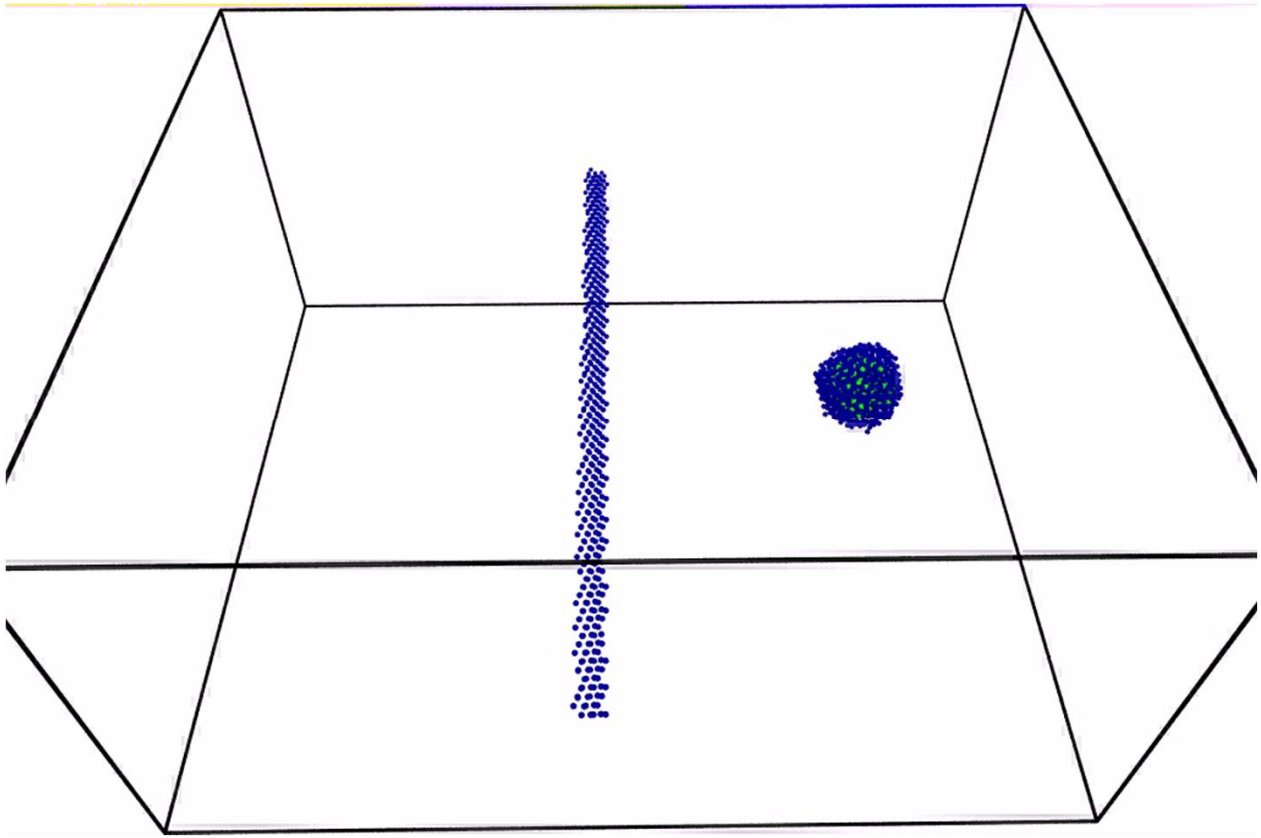


Fig. 1. Change in the free energy of SIA clusters of different sizes estimated for $T = 640$ K.

[D. Terentyev et al, Journal of Nuclear Materials 393 (2009) 30–35]

Dislocation slow-down: precipitates

- Also obstacles slow down dislocations
- Example: cementite Fe_3C precipitate and edge dislocation in Fe:



[F. Granberg, to be published (2014)]

The state of the art

- Overall, the current state of the art of knowledge of irradiation and dislocations can be summarized as

1. Irradiation is well known to generate dislocations both directly and by migration
2. The nature of the dislocations cannot be fully reliably predicted – different MD potentials give different results
3. Dislocations are known to be mobile, but the mobility is slowed down by impurities, alloying elements and obstacles in complex ways that are poorly known
4. After long irradiation, the dislocation buildup hardens metals, but the meso- and macroscale mechanisms are not understood
    - Combined MD and DDD work under way attempting to do that

What should you have learned from this section?

- You know the basics of dislocation structure and mobility (irradiation or not)
- You know that dislocations can form directly in collision cascades, or via atom migration
- You know that a nearby surface can enhance dislocation loop production
- You also realize that also more complex 3D defects like SFT's dislocation can be formed directly by irradiation
- You know how irradiation creates small dislocation loops, and that can slow down the mobility of bigger dislocations
- You know that irradiation effects on dislocations is not actually understood yet, and subject to ongoing research