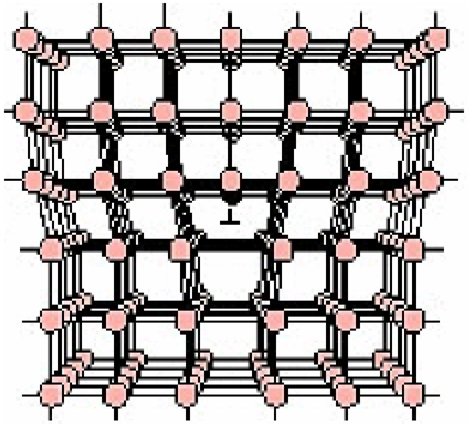
Ch. 4: Imperfections in Solids Part 2

Dr. Feras Fraige

Dislocations—Linear Defects

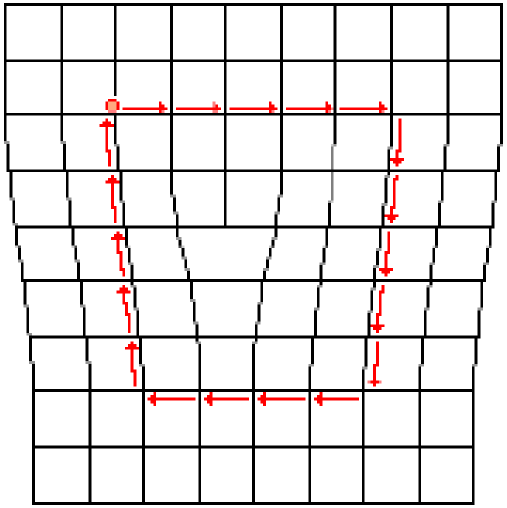
- **Dislocations are linear defects: the interatomic bonds are** significantly distorted only in the immediate vicinity of the dislocation line. This are called the **dislocation core.**
- Dislocations also create small elastic deformation the lattice at large distances.
- Dislocations are very important in mechanical properties of material (Chapters 6, 7, 8). Introduction/discovery of dislocations in 1934 by Taylor, Orowan and Polyani marked the beginning of our understanding of mechanical properties of materials.

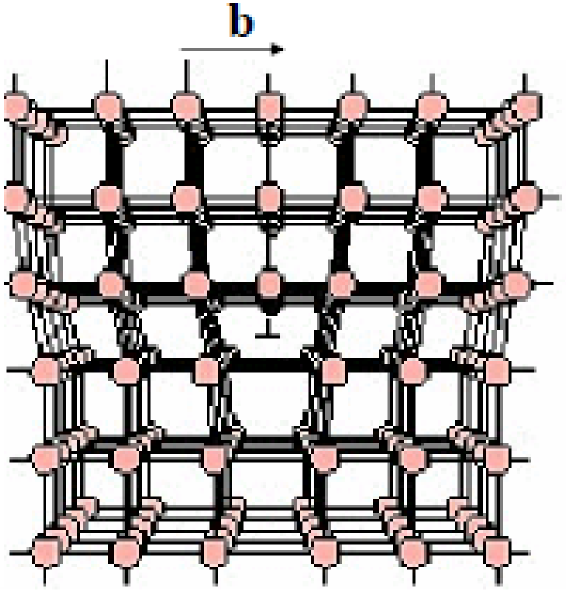


Description of Dislocations—Burgers Vector

- To describe the size and the direction of the lattice distortion caused by a dislocation we should introduce so called **Burgers vector b. To find the Burgers vector, we** should make a circuit from atom to atom counting the same number of atomic distances in all directions. If the circuit encloses a dislocation it will not close. The vector that closes the loop is the Burgers vector **b.**

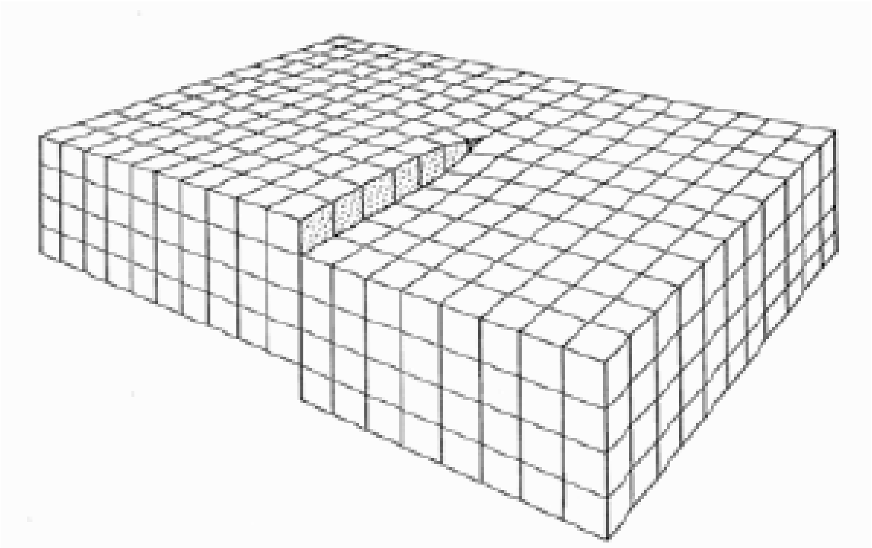
Dislocations shown here have Burgers vector directed perpendicular to the dislocation line. These dislocations are called **edge dislocations.**

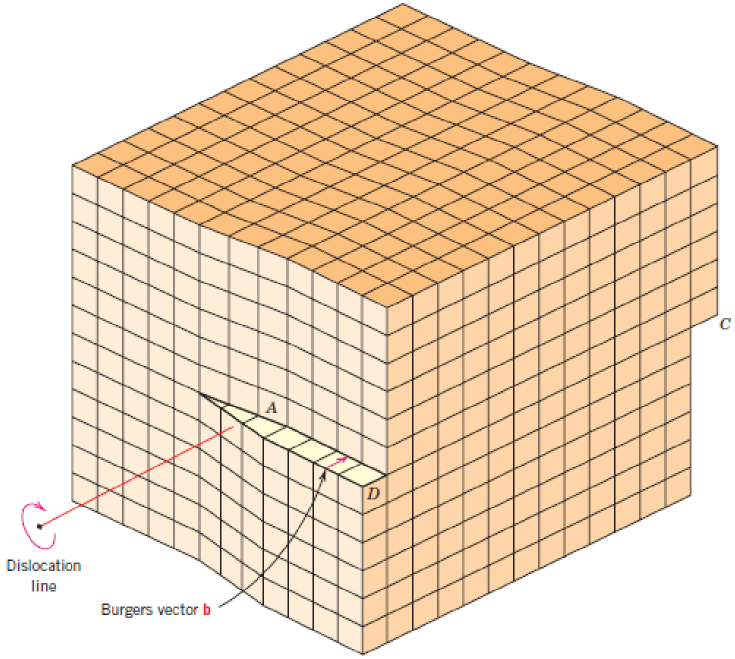




Edge and screw dislocations

- Dislocations shown in previous slide are **edge dislocations.**
- They have Burgers vector directed perpendicular to the dislocation line.
- There is a second basic type of dislocation, called **screw**
- **dislocation. The screw dislocation is parallel to the** direction in which the crystal is being displaced or sheared (Burgers vector is parallel to the dislocation line).



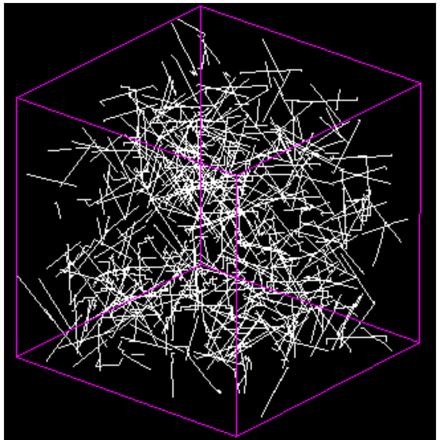


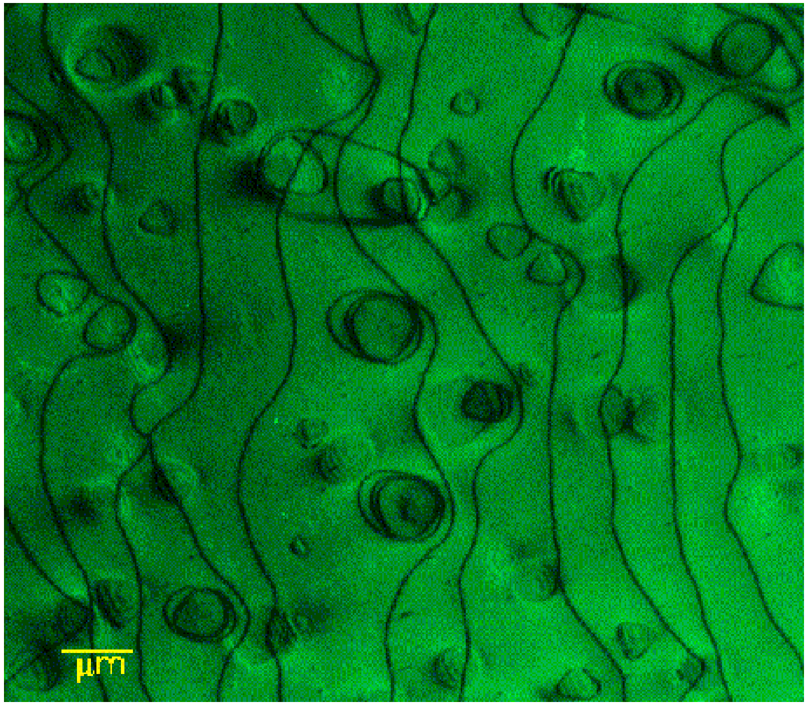
Mixed/partial dislocations

- The exact structure of dislocations in real crystals is usually more complicated than the ones shown in this pages. Edge and screw dislocations are just extreme forms of the possible dislocation structures. Most dislocations have mixed edge/screw character.
- To add to the complexity to real defect structures, dislocation are often split in "partial“ dislocations that have their cores spread out over a larger area.

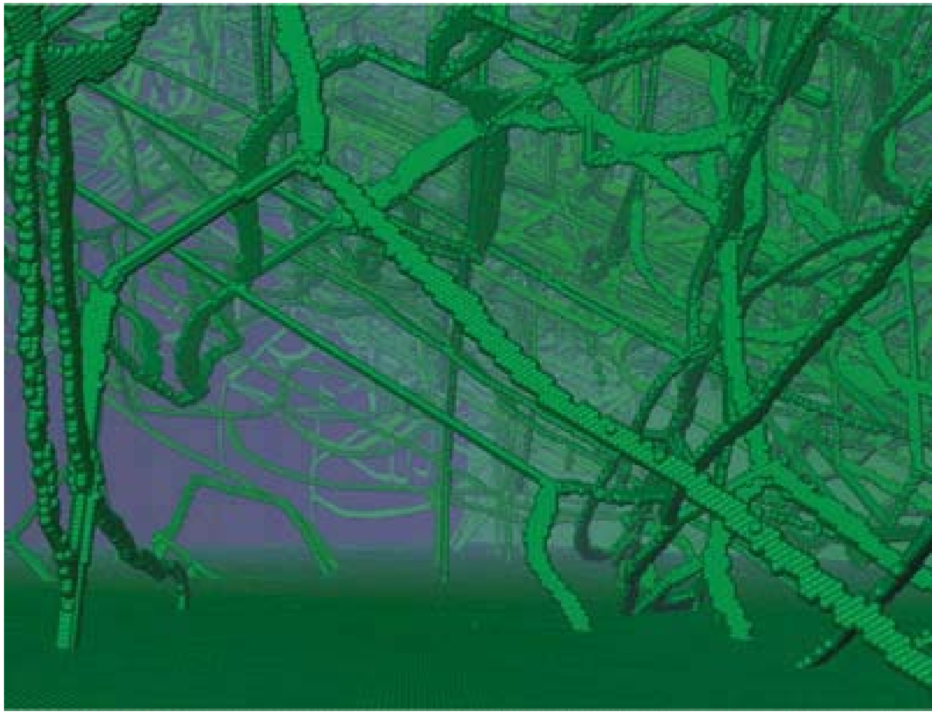
Where do dislocations come from ?

- The number of dislocations in a material is expressed as the **dislocation density - the total dislocation length per unit volume** or **the number of dislocations intersecting a unit area**. Dislocation densities can vary from 10^5 cm^{-2} in carefully solidified metal crystals to 10^{12} cm^{-2} in heavily deformed metals.
- Most crystalline materials, especially metals, have dislocations in their as-formed state, mainly as a result of stresses (mechanical, thermal...) associated with the forming process.
- The number of dislocations **increases** dramatically during plastic deformation (Ch.7). Dislocations spawn from existing dislocations, grain boundaries & surfaces





Dislocations in Ni (the dark lines and loops), transmission electron microscopy image, Manchester Materials Science Center.



Atomistic simulation of work-hardening in a FCC solid, IBM-LLNL collaboration.

Planar (interfacial) defects

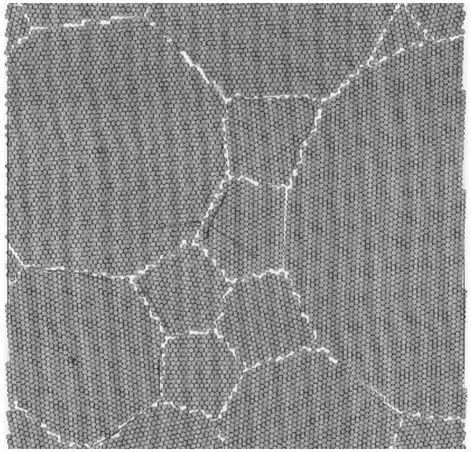
External Surfaces

- Surface atoms have unsatisfied atomic bonds, and higher energies than the bulk atoms ⇒ Surface energy, γ (J/m2)
- Minimization of surface areas reduces the energy of the system (e.g. liquid drop)
- Solid surfaces can “reconstruct” to satisfy atomic bonds at surfaces.

Planar (interfacial) defects

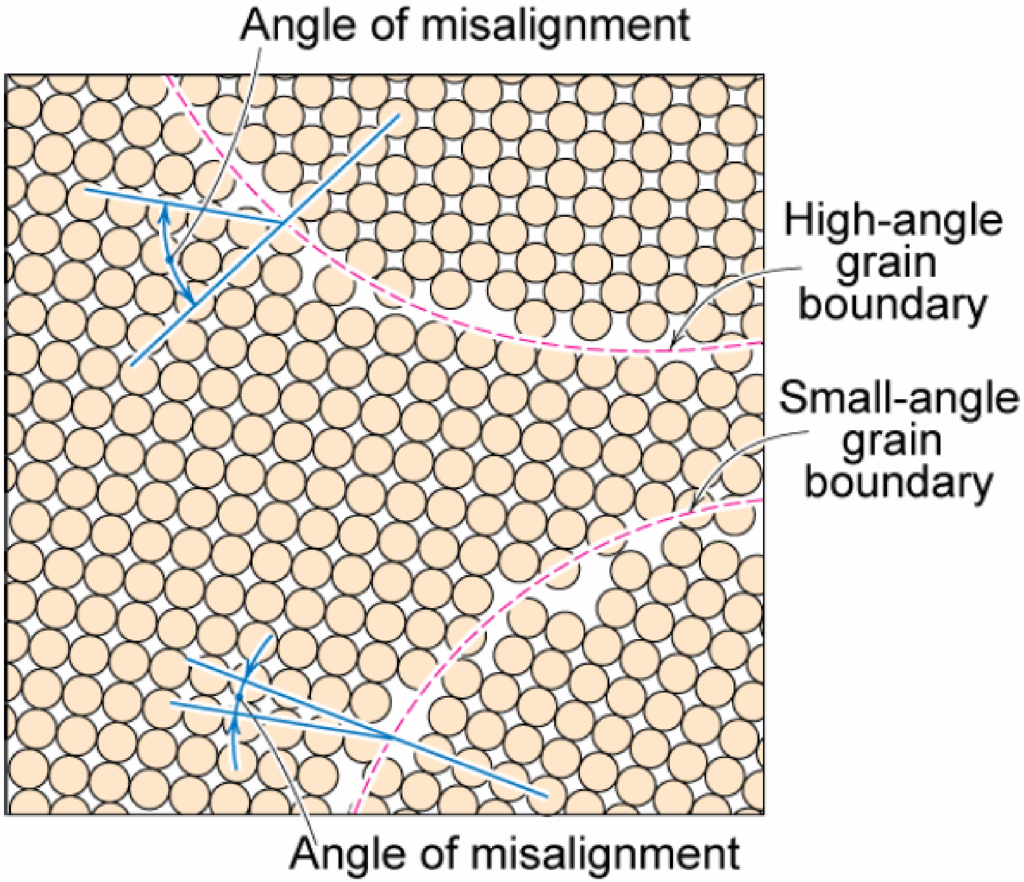
Grain Boundaries

- Polycrystalline material comprised of many small crystals or grains. The grains have different crystallographic orientation. There exist atomic mismatch within the regions where grains meet. These regions are called **grain boundaries.**
- Surfaces and interfaces have structure that is different from the bulk and can be reactive → impurities tend to segregate there.
- Since energy is associated with interfaces, grains tend to grow in size at the expense of smaller grains to minimize energy. This occurs by diffusion (Chapter 5), which is accelerated at high temperatures.



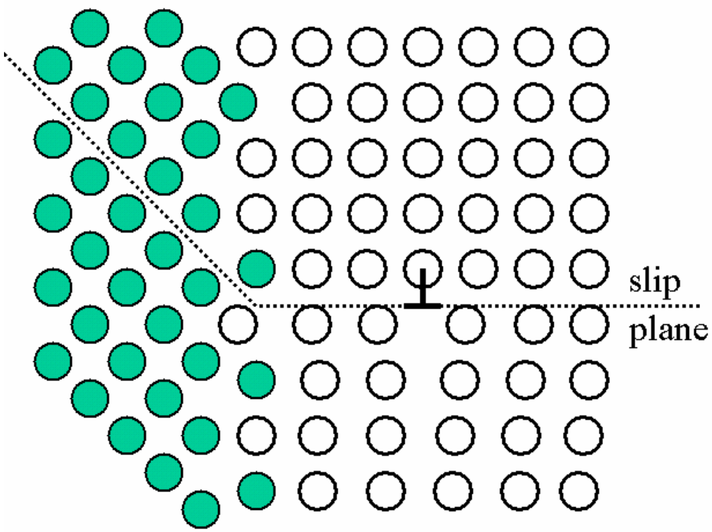
High and low angle grain boundaries

- Depending on misalignments of atomic planes between adjacent grains we can distinguish between the low and high angle grain boundaries (as shown below).



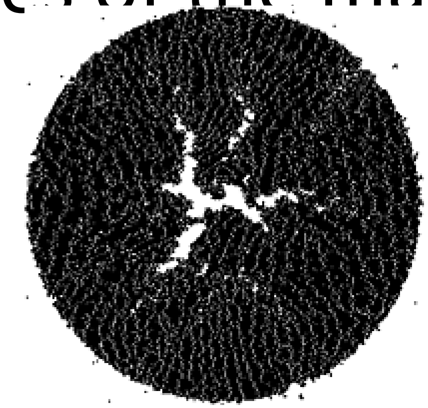
Interaction between dislocations and grain boundaries

- Motion of dislocations can be impeded by grain boundaries – increase of the force needed to move then (strengthening the material).
- Grain boundary present a barrier to dislocation motion: slip plane discontinues or change orientation.
- Small angle grain boundaries are not very effective in blocking dislocations.
- High-angle grain boundaries block slip and increase strength of the material. A stress concentration at end of a slip plane may trigger new dislocations in an adjacent grain.



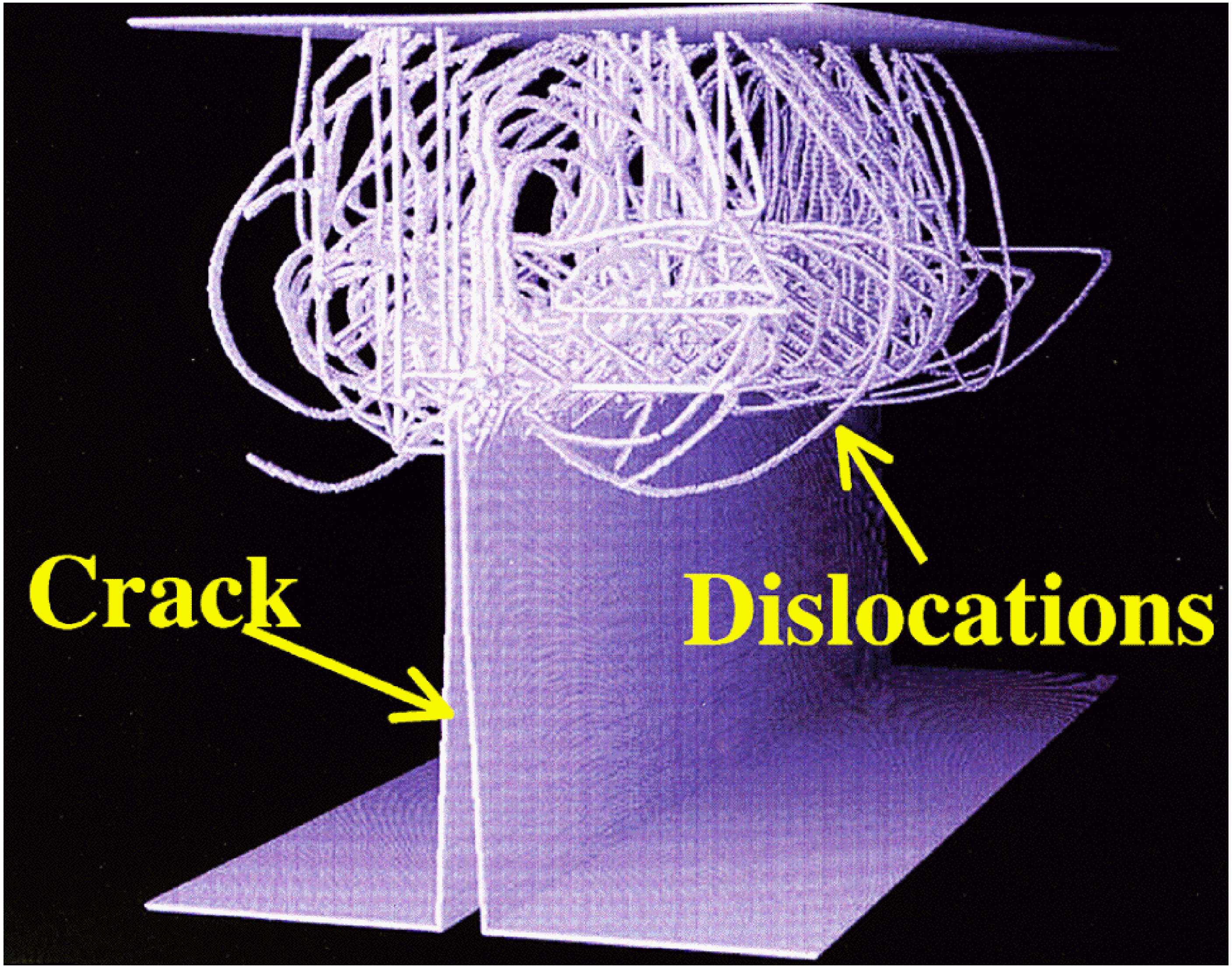
Bulk or volume defects

- **Pores**
- **Cracks**
- **Foreign inclusions**
- Presence of volume defects can greatly affect electrical, mechanical, thermal, and optical properties of the material.



A cluster of microcracks in a melanin granule irradiated by a short laser pulse.

Atomistic simulation of crack propagation



Atomic Vibrations

- Thermal energy (heat) causes atoms to vibrate.
- Vibration amplitude increases with temperature.
- Melting occurs when vibrations are sufficient to rupture large number of atomic bonds.
- Vibrational frequency ~ 10^{13} Hz (10^{13} vibrations per second)

Summary

Make sure you understand language and concepts:

- Alloy
- Atom percent
- Atomic vibration
- Boltzmann's constant
- Burgers vector
- Composition
- Dislocation line
- Edge dislocation
- Grain boundary
- Imperfection
- Impurity
- Interstitial solid solution
- Microstructure
- Point defect
- Screw dislocation
- Self-interstitial
- Solid solution
- Solute
- Solvent
- Substitutional solid solution
- Vacancy
- Weight percent