The University Of Sheffield.

EEE 6212
Semiconductor Materials

Lecture 6: Lattice defects

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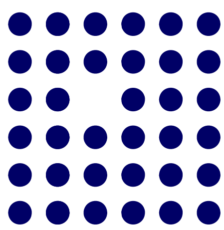
- classification of lattice defects according to their dimensionality
- point defects
- line defects
- two-dimensional lattice defects
- three-dimensional defects

classification of lattice defects

dimensionality and types of lattice defects:

- 0D or point defects: vacancies, dopants, interstitials, Schottky defects, Frenkel-pairs, colour centres
- 1D or line defects: dislocations
- 2D defects: special grain boundaries (anti-phase, inversion domain), stacking faults
- 3D defects: pores, precipitates, clusters, general phase boundaries

point defects (0D): types



- vacancies: atom missing on lattice site
- dopants: foreign atom on lattice site
- interstitials: additional atom between lattice sites
- Schottky defects: vacancy left behind by atom having moved to the surface of the crystal
- Frenkel-pairs: thermal vacancy & interstitial
- colour centres: electron on interstitial site

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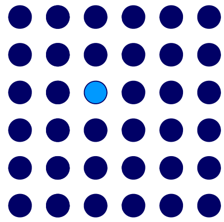

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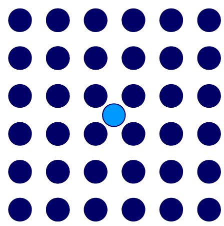

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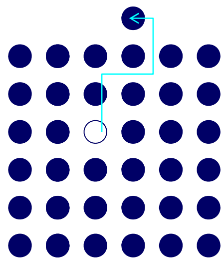

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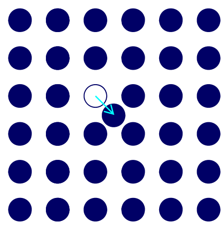

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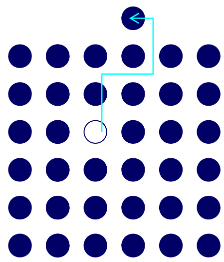
point defects (0D): formation



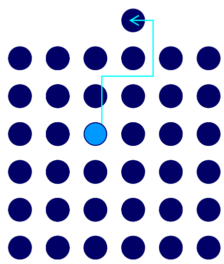
- thermal anneal (heating)

  (e.g. hardening of metal alloys)
- irradiation (e.g. by X-rays)

  (e.g. steels for nuclear reactors)
- doping by diffusion from surface

  (e.g. for solid state electrolytes)
- doping by ion implantation and anneal (e.g. for pn diodes for electronics)

example of doping by ion implantation and annealing



principle of diffusion:

- particle current density: $\underline{j}=-D \text{ grad } n$
- continuity equation: $\partial n/\partial t = -\text{div } \underline{j}$

-> Fick's law of diffusion: $\partial n/\partial t = D \text{ div grad } n$

in 1 dimension (x): $\partial n/\partial t = D\, \partial^2 n/\partial x^2$

with diffusion coeff. $D=D_0 \exp(-E/kT)$

(D_0= diffusion constant, k=Boltzmann const., T=temp.)

solutions depend on boundary conditions:

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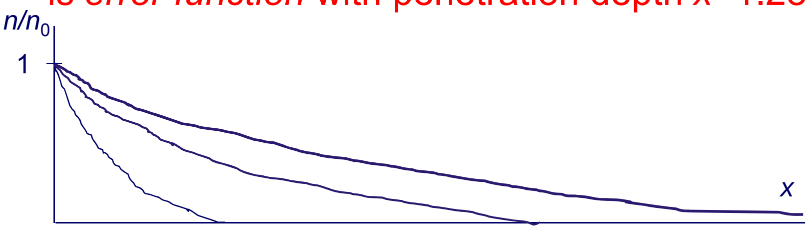
example of doping by surface diffusion and annealing

a) constant concentration on the surface:

$n(x,0)=0$ & $n(0,t)=n_0=\text{const}$

-> $n(x,t)=n_0\,[1-2/\sqrt{\pi}\int_0^a \exp(-u^2)\,du]$ with $a=x/(2\sqrt{Dt})$

is *error function* with penetration depth $x=1.28\sqrt{Dt}$



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example of doping by surface diffusion and annealing

b) constant number of dopant atoms on the surface:

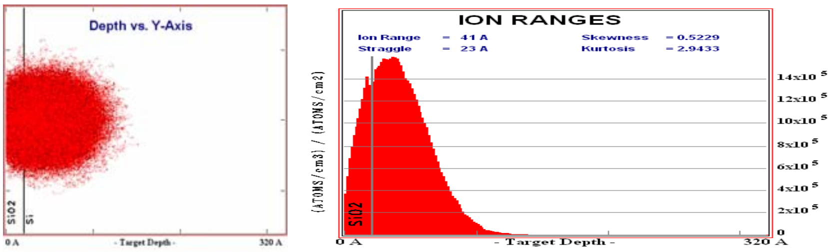
$n(x,0)=0$ for $x>0$, $N(0,0)=n_0 d\,\delta(x)$ for $x=0$ & $n(0,0)=n_0$

-> $n(x,t)=n_0 d/(\sqrt{\pi Dt})\exp-[x^2/(4Dt)]$

is *Gauss function* with depth $x=2\sqrt{Dt}>>d$, area $n_0 d$

example of doping by ion implantation and annealing

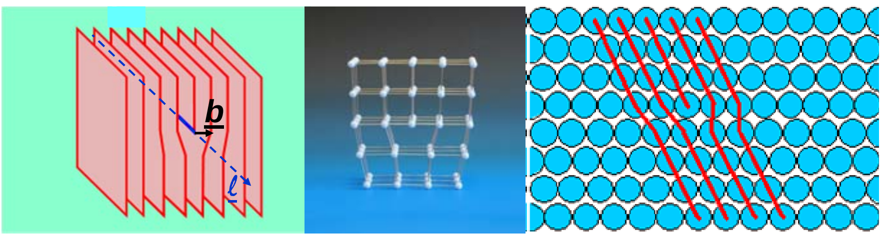
c) need ion implantation to achieve max. number of dopants is reached below the surface



B implantation (from left) of Si with native SiO_2 on surface

line defects (1D): dislocations

edge dislocation

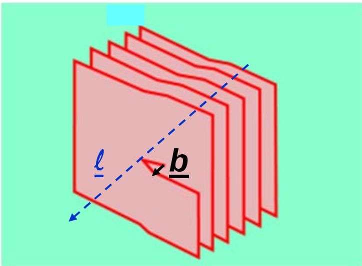


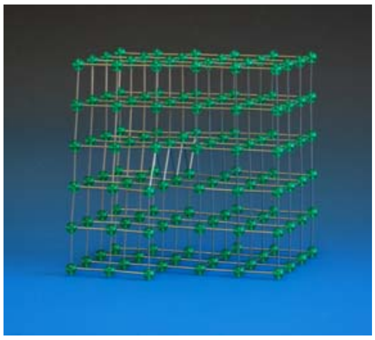
model: additional atomic plane inserted, yielding step

definition: line direction perpendicular to Burgers vector, which describes length & direction of a closure fault and can never end within a crystal but only on its surface!

line defects (1D): dislocations

screw dislocation



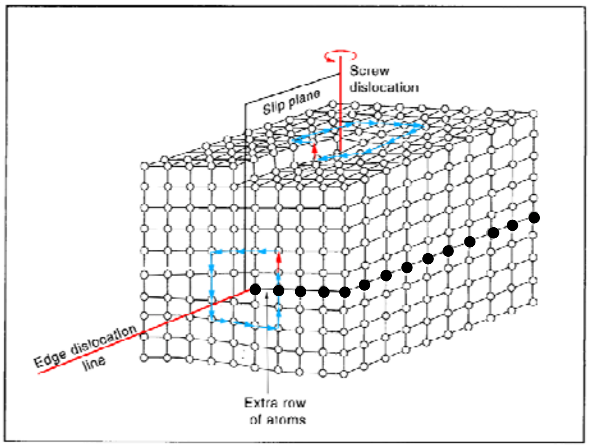


model: twisted atomic planes, yielding spiral staircase

definition: line direction parallel to Burgers vector

line defects (1D): dislocations

mixed dislocation: ***b***=const but line direction changes

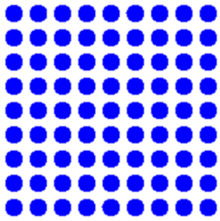


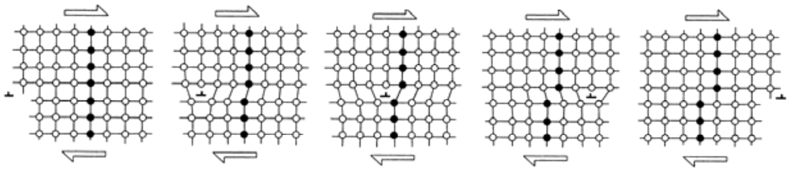
line defects (1D): dislocations

how an edge dislocation moves:

animation from:

www.tf.uni-kiel.de/matwis





Migration of dislocation

Crystal shape has changed without mechanical fracturing or loss of crystal structure

line defects (1D): dislocations

elastic energy per length stored within a screw dislocation:

consider cylinder with embedded screw dislocation where torus of radius *r* and thickness d*r* is displaced along dislocation line by *b*.

If *G*=shear modulus, then

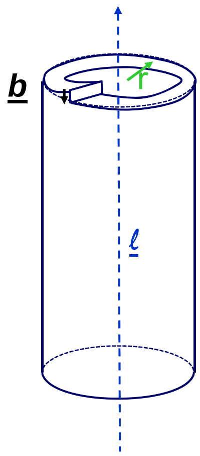
-> shear angle: $\alpha = b/(2\pi r)$

-> shear stress: $\tau = G\alpha = Gb/(2\pi r)$

-> elastic energy stored per length and volume:

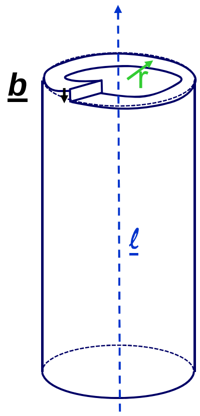
$dE/dV = G \int \alpha \, d\alpha$ and $dV = 2\pi r dr$

-> $dE = G \int \alpha \, d\alpha \, dV = G \, \alpha^2/2 \, dV = Gb^2/(4\pi) \, 1/r \, dr$



line defects (1D): dislocations

elastic energy per length stored within a screw dislocation:



-> $dE = G \int \alpha \, d\alpha \, dV = G \, \alpha^2/2 \, dV$

$= Gb^2/(4\pi) \, 1/r \, dr$

-> $E = \int dE$

$= Gb^2/(4\pi) \; \ln r \Big|_{r_i \approx 5b}^{r_o}$

$= Gb^2/(4\pi) \ln r_o/r_i$

$\approx ½ \, Gb^2$

where, b=length of Burgers vector,

r_o = outer radius of cylinder around screw dislocation, $r_i \approx 5b$

line defects (1D): dislocations

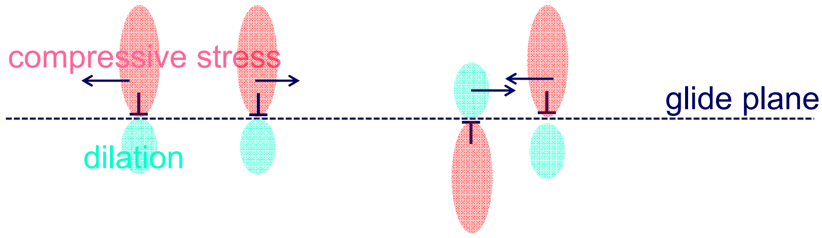
total energy: $E\ell = Gb^2\ell/(4\pi) \ln r_o/r_i \approx ½ \, Gb^2\ell$

(note: edge dislocations: similar apart from a factor of $1/(1-\nu)$ where ν is Poisson ratio)

The energy of such a dislocation is ~5-8eV, far too large to be produced thermally at any temperature. The only way to form them is by force, i.e.: deformation, stress at surfaces & interfaces or by dislocation reactions (multiplication).

line defects (1D): dislocations

Because of $E \propto b_{tot}^2$, and $\underline{\boldsymbol{b}}_{tot}=\Sigma\ \underline{\boldsymbol{b}}_i$, dislocations with the same Burgers vector direction repel each other, (often leading to equidistant spacings within a plane) while those with opposite Burgers vector attract each other (-> annihilation).



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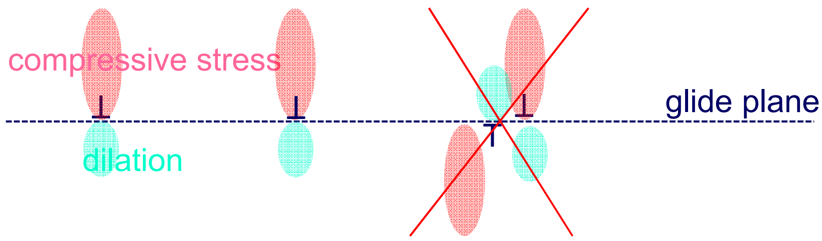

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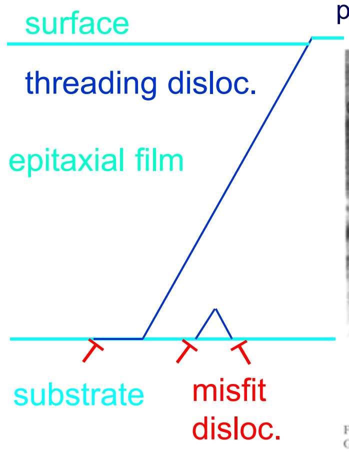
line defects (1D): dislocations

Formation of dislocation networks that can attract impurities.

side view (sketch)



top view: dislocations decrease optical output of GaAs (DB Holt, IoP Conf Ser. 134 (1993) 661)

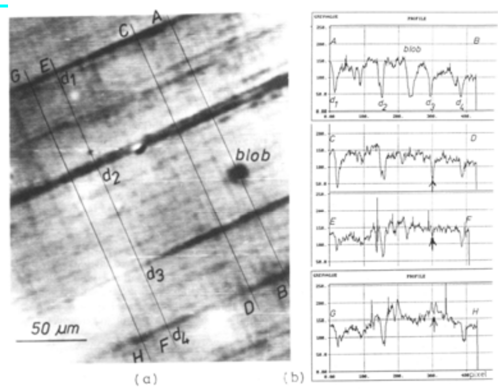


Figure 3. (a) part of a digitized 512×512 pixel ECL image of beam-induced dislocations in GaAs and (b) a number of CL intensity profiles for the scan lines marked in (a).

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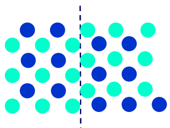
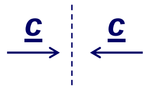
2D defects



- stacking faults
- anti-phase domains
- inversion domains in non-centrosymmetric crystals
- other special (flat) grain boundaries



3D defects

- small pores formed by vacancy agglomeration
- clusters of atoms formed by segregation
- precipitates (of foreign atoms) of all forms & shapes
- general phase boundaries