

FYS3410 - Vår 2016 (Kondenserte fasers fysikk)

<http://www.uio.no/studier/emner/matnat/fys/FYS3410/v16/index.html>

**Pensum: Introduction to Solid State Physics
by Charles Kittel (Chapters 1-9 and 17, 18, 20)**

Andrej Kuznetsov

delivery address: Department of Physics, PB 1048 Blindern, 0316 OSLO

Tel: +47-22857762,

e-post: andrej.kuznetsov@fys.uio.no

visiting address: MiNaLab, Gaustadaleen 23a

2016 FYS3410 Lectures (based on C.Kittel's Introduction to SSP, Chapters 1-9, 17,18,20)

Module I – Periodic Structures and Defects (Chapters 1-3, 20)

M18/1: 9-12 am	Introduction. Crystal bonding. Periodicity and lattices, Brag diffraction and Laue condition, reciprocal space	3h
<i>W20/1 cancelled</i>		
M25/1: 9-12 am	Ewald construction, interpretation of a diffraction experiment , Brag planes, and Brillouin zones	3h
<i>W27/1 cancelled</i>		
M01/2: 10-12 am	Elastic strain and structural defects in crystals	2h
W03/2: 9-10 am	Atomic diffusion in solids	1h
M08/2: 10-12 am	Summary of Module I	2h

Module II – Phonons (Chapters 4 and 5)

W10/2: 9-10 am	Vibrations in monoatomic and diatomic chains of atoms	1h
M15/2: 10-12am	Periodic boundary conditions, phonons and density of states (DOS)	2h
W17/2: 9-10 am	Planck distribution	1h
M22/2 : 10-12am	Lattice heat capacity: Dulong-Petit, Einstein, and Debye models	2h
<i>W24/2 cancelled</i>		
M29/2: 9-12am	Comparison of different models for lattice heat capacity, thermal conductivity with phonons	3h
W02/3: 9-10 am	Thermal expansion	1h
M07/3: 10-12am	Summary of Module II.	2h

Module III – Electrons (Chapters 6, 7, 18 - pp.528-530, and Appendix D)

W09/3: 9-10 am	Free electron gas (FEG) versus free electron Fermi gas (FEFG)	1h
M14/3: 10-12am	DOS of FEFG in 3D. Effect of temperature – Fermi-Dirac distribution	2h
W16/3: 9-10 am	Heat capacity of FEFG in 3D	1h
W30/3: 9-10 am	DOS in 2D - quantum wells	1h
M04/4: 10-12am	DOS in 1D and 0D, i.e. quantum wires and quantum dots; transport properties of electrons	2h
W06/4: 9-10 am	Origin of the energy band gap	
M11/4: 10-12am	Nearly free electron model. Kronig-Penney model. Empty lattice approximation.	2h
W13/4: 9-10 am	Number of orbitals in a band	1h
M18/4: 10-12am	Summary of Module III.	2h

Module IV – Semiconductors and interfaces (Chapters 8, 9-pp 223-231, 17)

W20/4: 9-10 am	Metals versus semiconductors. Surfaces and interfaces.	1h
M25/4: 9-12 am	Effective mass method.	3h
W27/4: 9-10 am	Intrinsic carrier generation – electrons and holes.	1h
M02/5: 9-12 am	Localized levels for hydrogen-like impurities – donors and acceptors. Doping.	3h
W04/5: 9-10 am	Carrier statistics in semiconductors	1h
M09/5: 9-12 am	p-n junctions	3h
W11/5: 9-10 am	Optoelectronic semiconductor properties and devices	1h
M18/5: 9-12 am	Device demonstrations. Summary of Module IV	3h

Repetition

M23/5 9-12 am	The course in a nutshell	2h
<i>W25/5, M30/5 and W1/6 cancelled</i>		

Exam during week 22 (tentatively 30-31/5)

Lecture 4: Atomic diffusion

- **Phenomenology of diffusion: describing diffusion in terms of diffusion flux**
- **Microscopic diffusion mechanisms**
- **Sb diffusion as a function of temperature as stress in Si/SiGe heterostructures**

Lecture 4: Atomic diffusion

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Diffusion

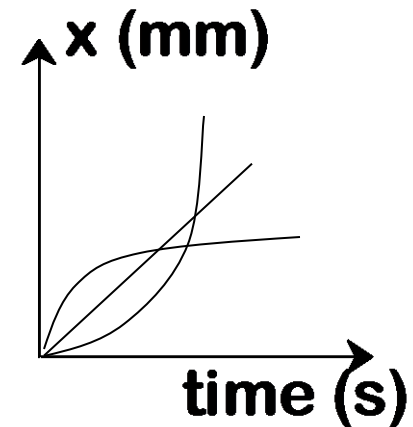
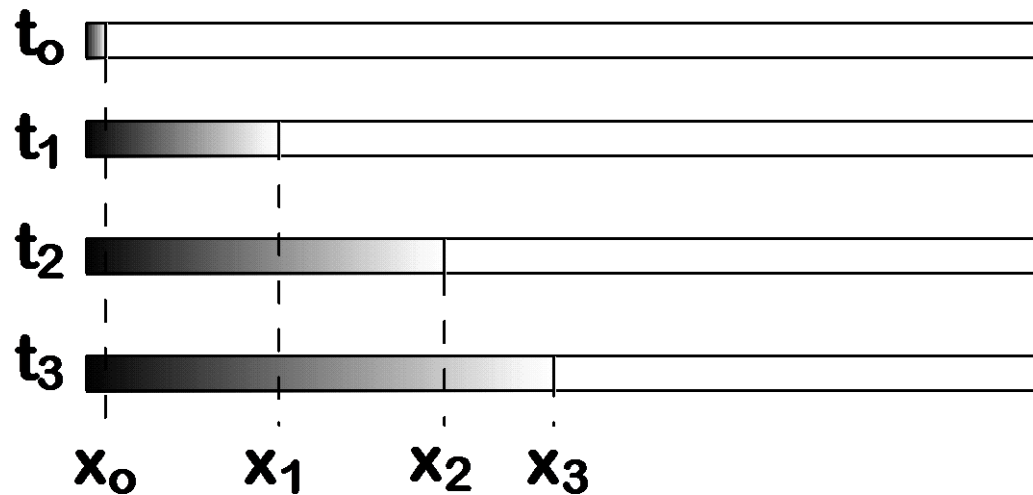
Phenomenon of material transport by atomic or particle transport from region of high to low concentration



- What forces the particles to go from left to right?
- Does each particle “know” its local concentration?
- Every particle is equally likely to go left or right!
- At the interfaces in the above picture, there are **more** particles going right than left → this causes an average “flux” of particles to the right!
- Largely determined by probability & statistics

Diffusion

- Glass tube filled with water.
- At time $t = 0$, add some drops of ink to one end of the tube.
- Measure the diffusion distance, x , over some time.

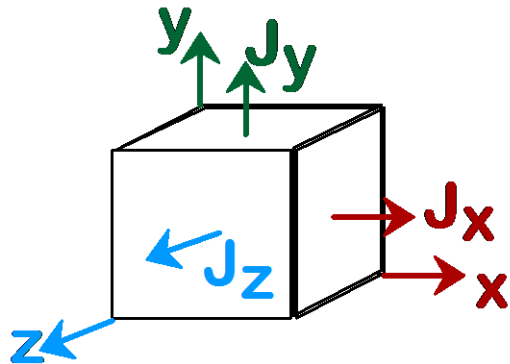


Describing diffusion in terms of diffusion flux

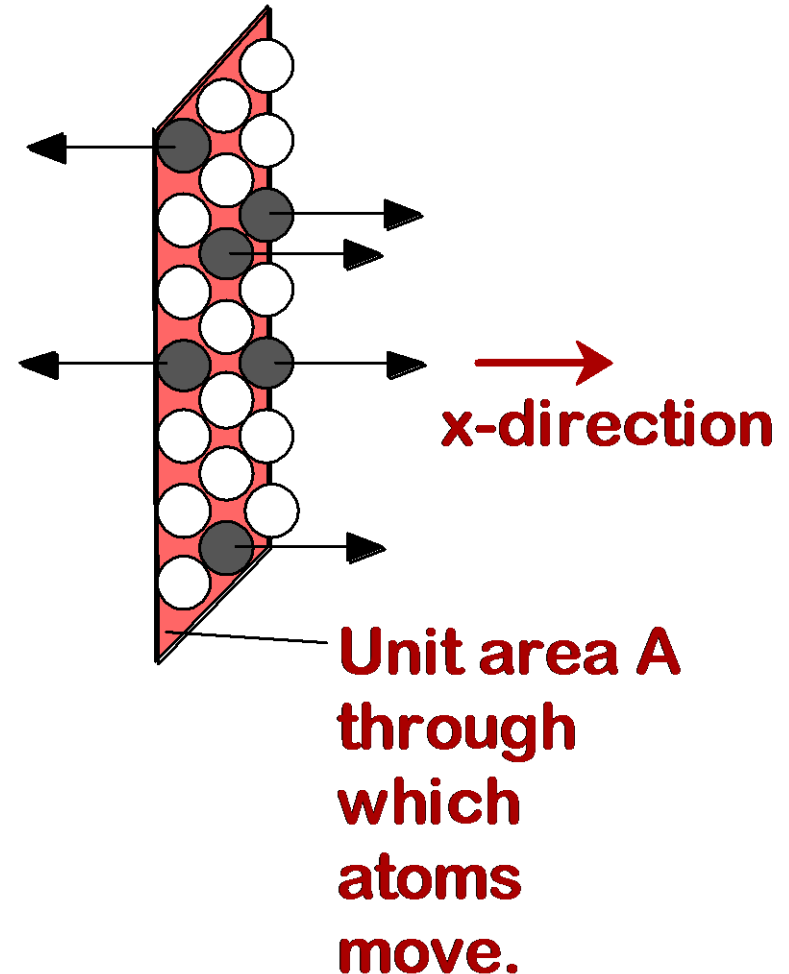
- **Flux**: amount of material or atoms moving past a unit area in unit time
Flux, $J = \Delta M / (A \Delta t)$

$$J = \frac{1 \, dM}{A \, dt} \Rightarrow \left[\frac{\text{kg}}{\text{m}^2 \text{s}} \right] \text{ or } \left[\frac{\text{atoms}}{\text{m}^2 \text{s}} \right]$$

- Directional Quantity

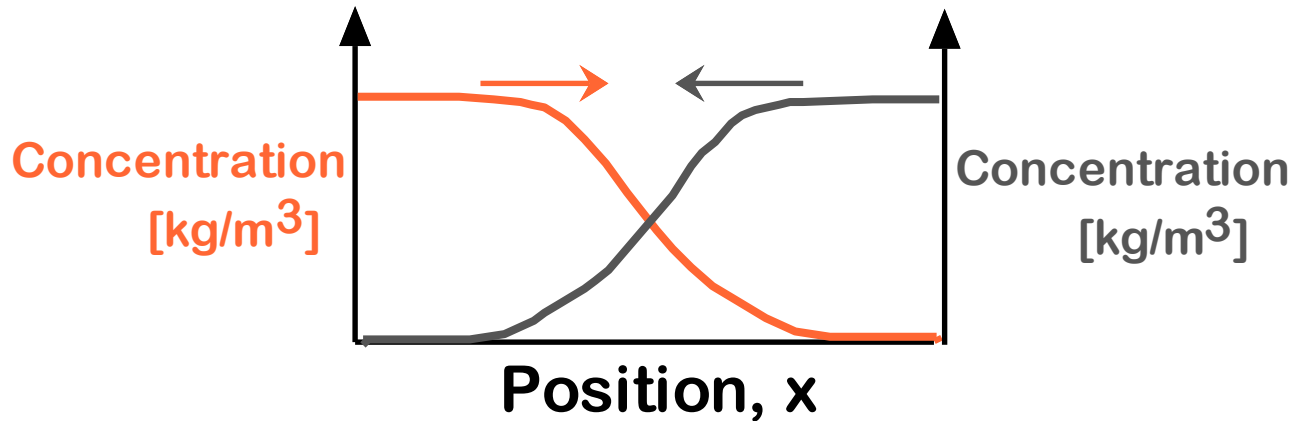


- Flux can be measured for:
 - vacancies
 - host (A) atoms
 - impurity (B) atoms



Describing diffusion in terms of diffusion flux

- Concentration Profile, $C(x)$: $[\text{kg}/\text{m}^3]$



- Fick's First Law:

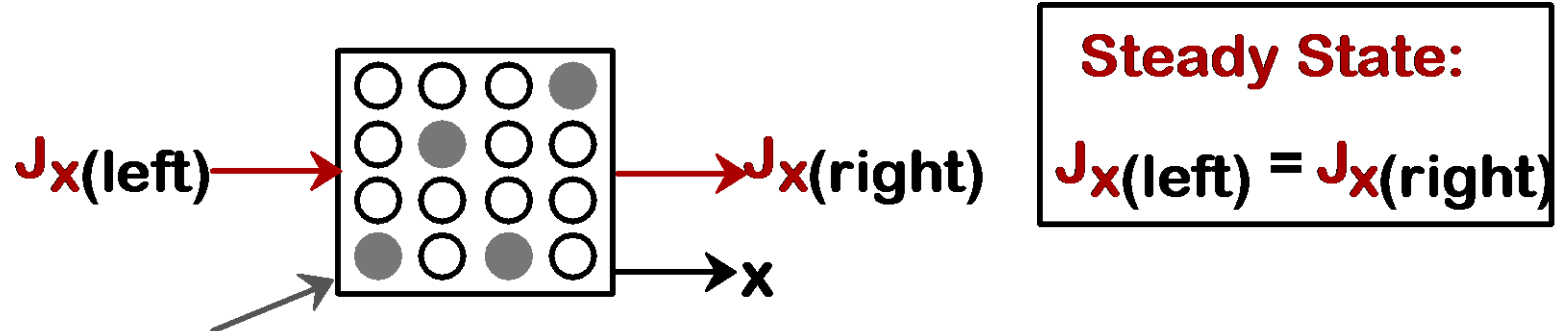
flux in x-dir.
 $[\text{kg}/\text{m}^2\text{-s}]$ → $J_x = -D \frac{dC}{dx}$

Diffusion coefficient $[\text{m}^2/\text{s}]$ → D

concentration gradient $[\text{kg}/\text{m}^4]$ → $\frac{dC}{dx}$

Describing diffusion in terms of diffusion flux

- **Steady State:** Steady rate of diffusion from one end to the other. Implies that the concentration profile doesn't change with time. Why?

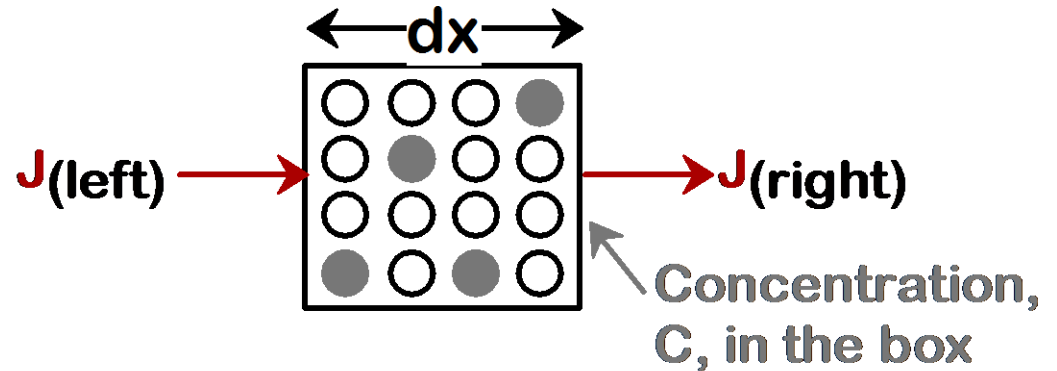


Concentration, C , in the box doesn't change w/time.

- Apply Fick's First Law: $J_x = -D \frac{dC}{dx}$
- If $J_x)_{\text{left}} = J_x)_{\text{right}}$, then $\left(\frac{dC}{dx} \right)_{\text{left}} = \left(\frac{dC}{dx} \right)_{\text{right}}$
- Result: the slope, dC/dx , must be constant (i.e., slope doesn't vary with position)!

Describing diffusion in terms of diffusion flux

- Concentration profile, $C(x)$, changes w/ time.



- To conserve matter:

$$\frac{J(\text{right}) - J(\text{left})}{dx} = -\frac{dC}{dt}$$

$$\frac{dJ}{dx} = -\frac{dC}{dt}$$

- Fick's First Law:

$$J = -D \frac{dC}{dx}$$

$$\frac{dJ}{dx} = -D \frac{d^2C}{dx^2} \quad (\text{if } D \text{ does not vary with } x)$$

equate

- Governing Eqn.:

$$\frac{dC}{dt} = D \frac{d^2C}{dx^2}$$

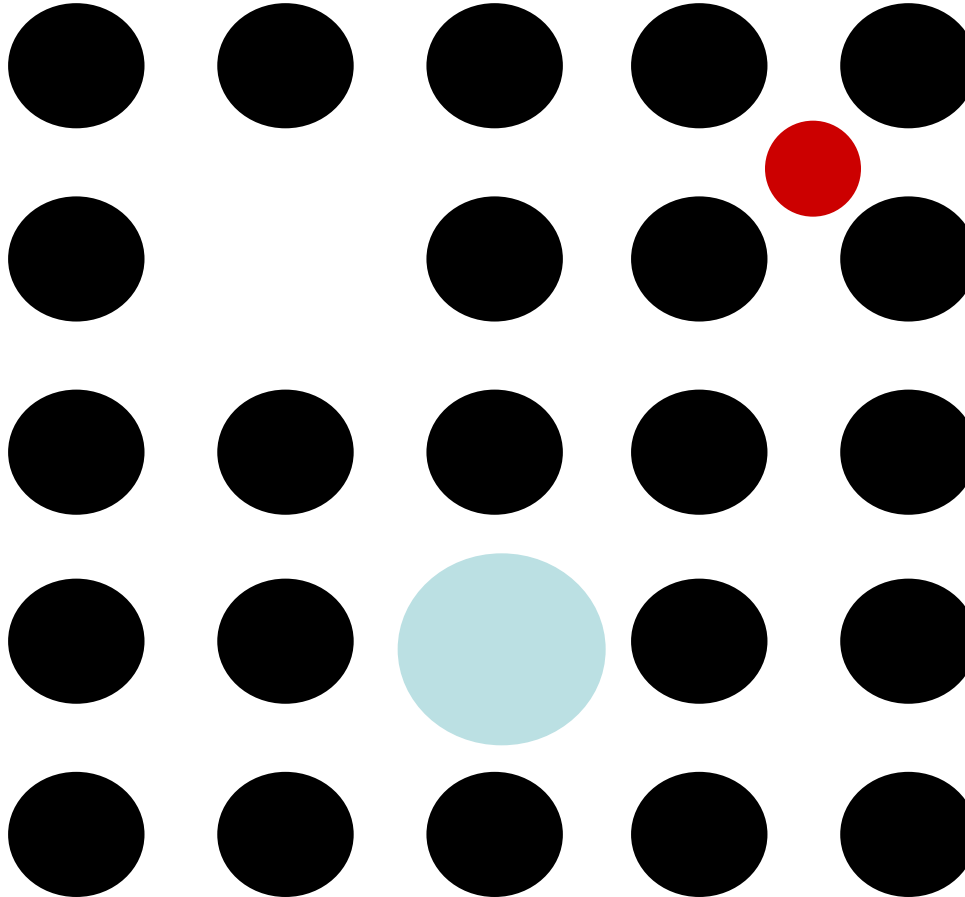
Fick's second law

Lecture 4: Atomic diffusion

- **Phenomenology of diffusion: describing diffusion in terms of diffusion flux**
- **Microscopic diffusion mechanisms**
- *Sb diffusion as a function of temperature as stress in Si/SiGe heterostructures*

Type of point defects

vacancy



**Interstitial
impurity**

**Substitutional
impurity**

Diffusion mechanisms

Diffusion at the atomic level is a step-wise migration of atoms from lattice site to lattice site

Conditions for diffusion:

- there must be an adjacent empty site
- atom must have sufficient energy to break bonds with its neighbors and migrate to adjacent site (“activation” energy)

Higher the temperature, higher is the probability that an atom will have sufficient energy

→ hence, diffusion rates increase with temperature

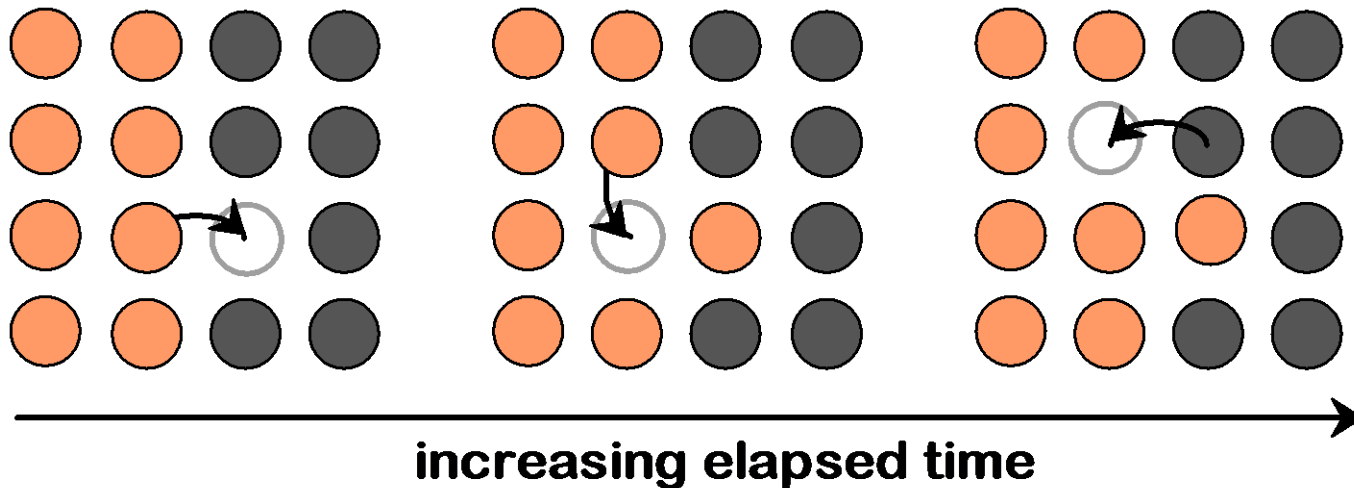
Types of atomic diffusion mechanisms:

- substitutional (through vacancies)
- interstitial

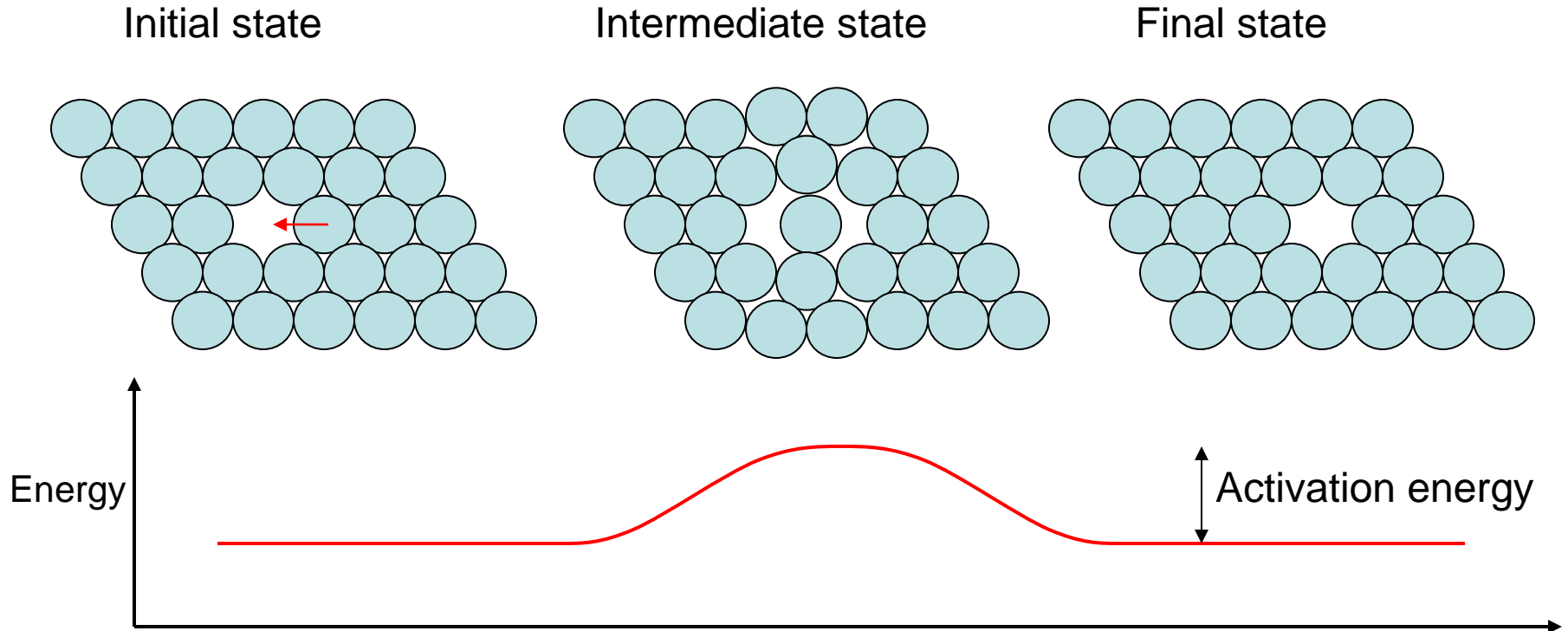
Diffusion mechanisms

Substitutional Diffusion:

- applies to substitutional impurities
- atoms exchange with vacancies
- rate depends on:
 - number of vacancies
 - temperature
 - activation energy to exchange.



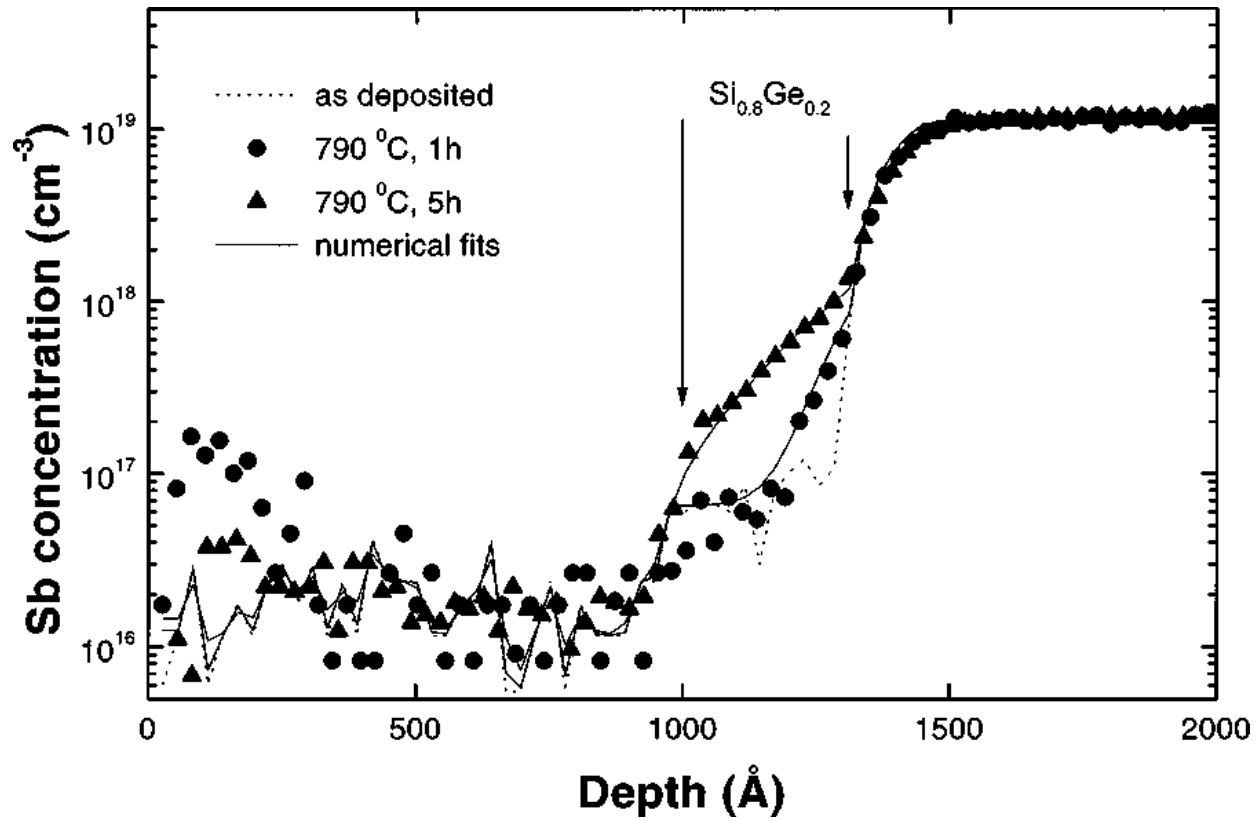
Diffusion mechanisms

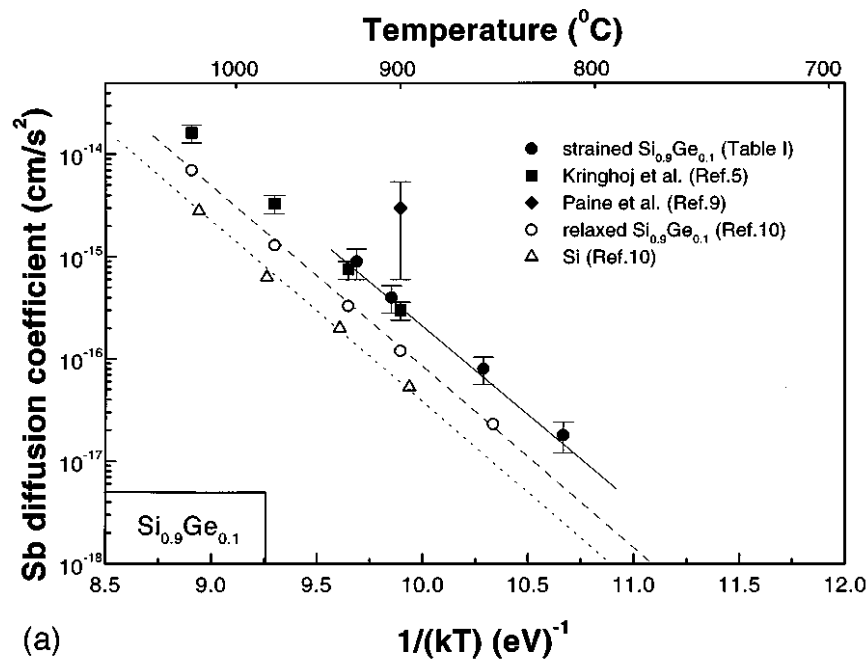


- Also called energy barrier for diffusion

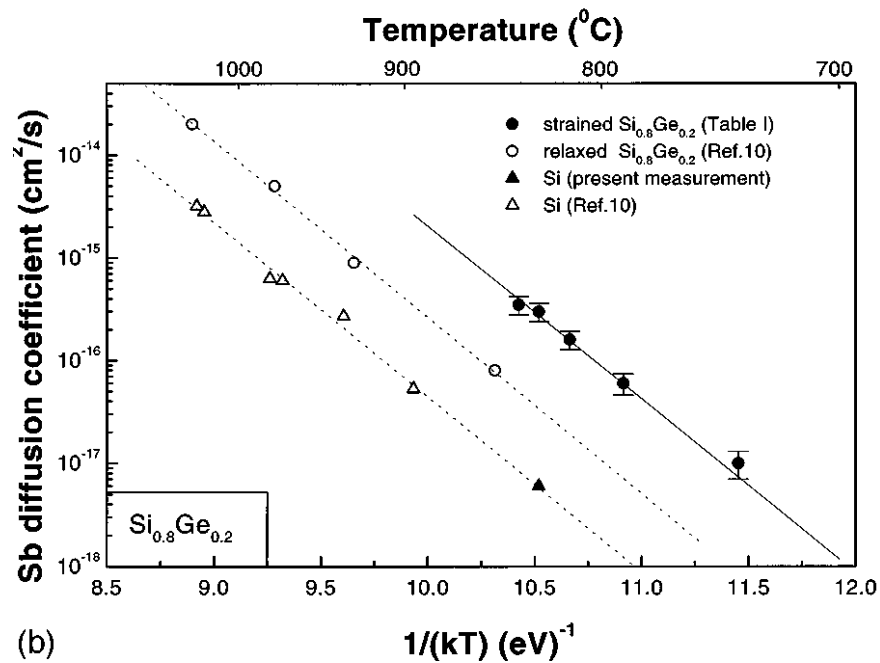
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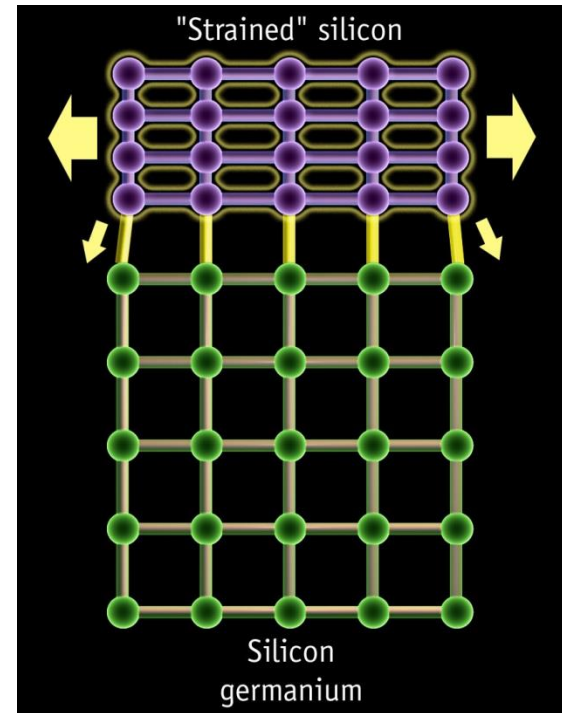
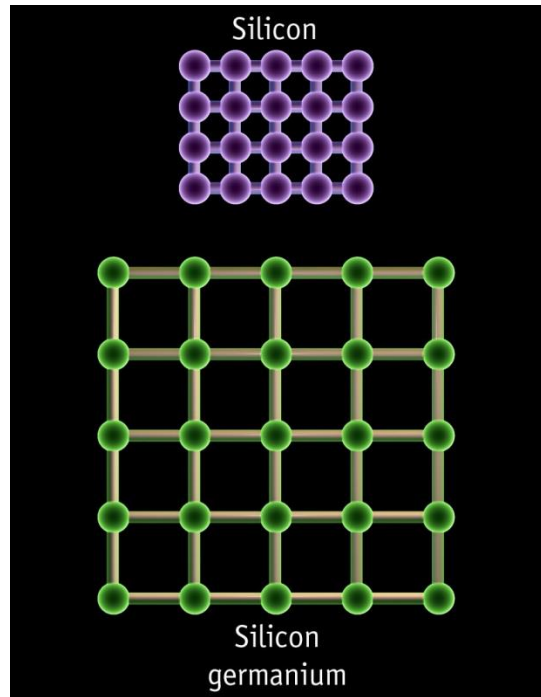


(a)



(b)

Strained silicon

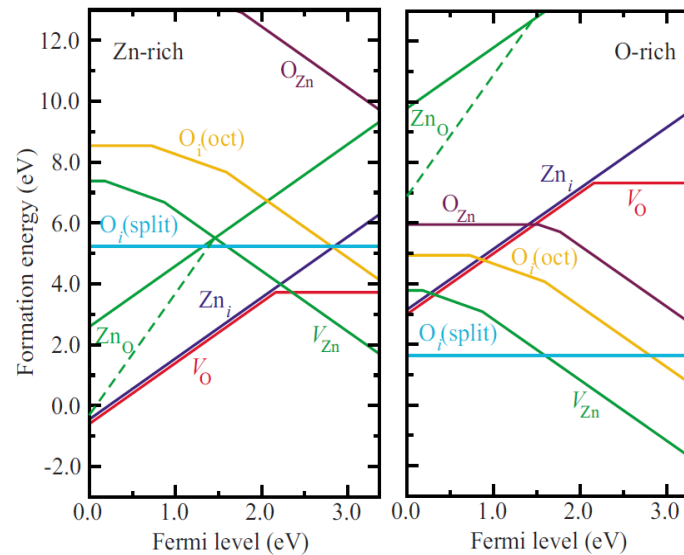


- How does it work?
- Basic idea: Change the lattice constant of material

Zn self-diffusion revealing V_{Zn} energetics

- astonishing progress is reached calculating intrinsic defect energetics in ZnO by *ab initio* methods, however the experimental verification is missing

from A. Janotti and C.G. Van de Walle, Phys.Rev. B 76 165202(2007)



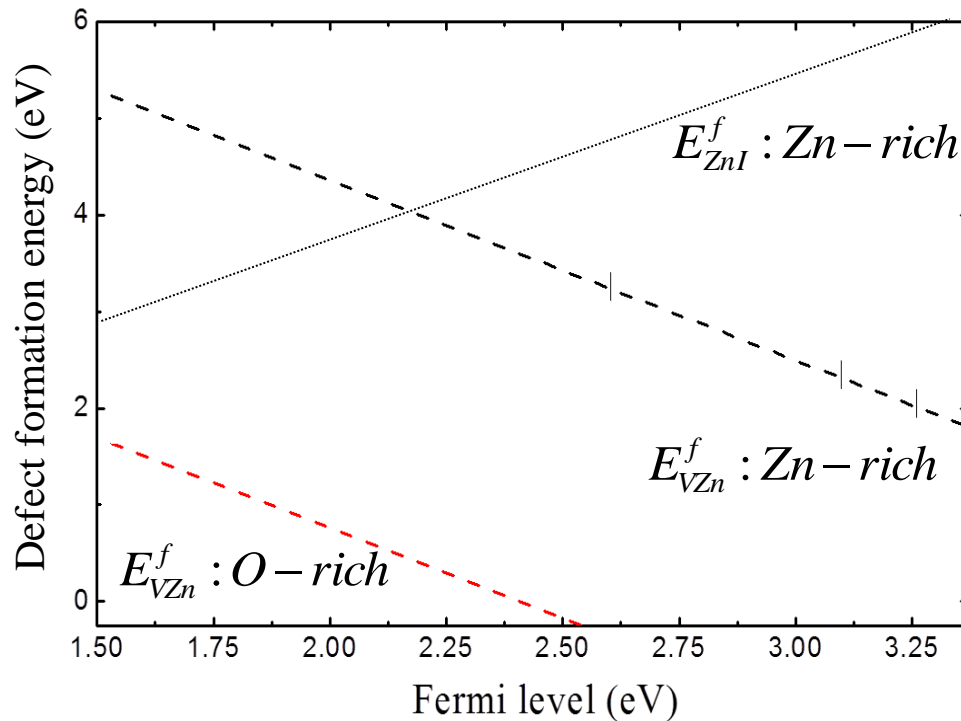
- Zn self-diffusion – as method assessing intrinsic defect energetics

$$D_{Zn}^V = D_0^V e^{-(E_{VZn}^f + E_{VZn}^m)/kT}$$

$$D_{Zn}^I = D_0^I e^{-(E_{ZnI}^f + E_{ZnI}^m)/kT}$$

Zn self-diffusion revealing V_{Zn} energetics

from A. Janotti and C.G. Van de Walle, Phys.Rev. B 76 165202(2007)



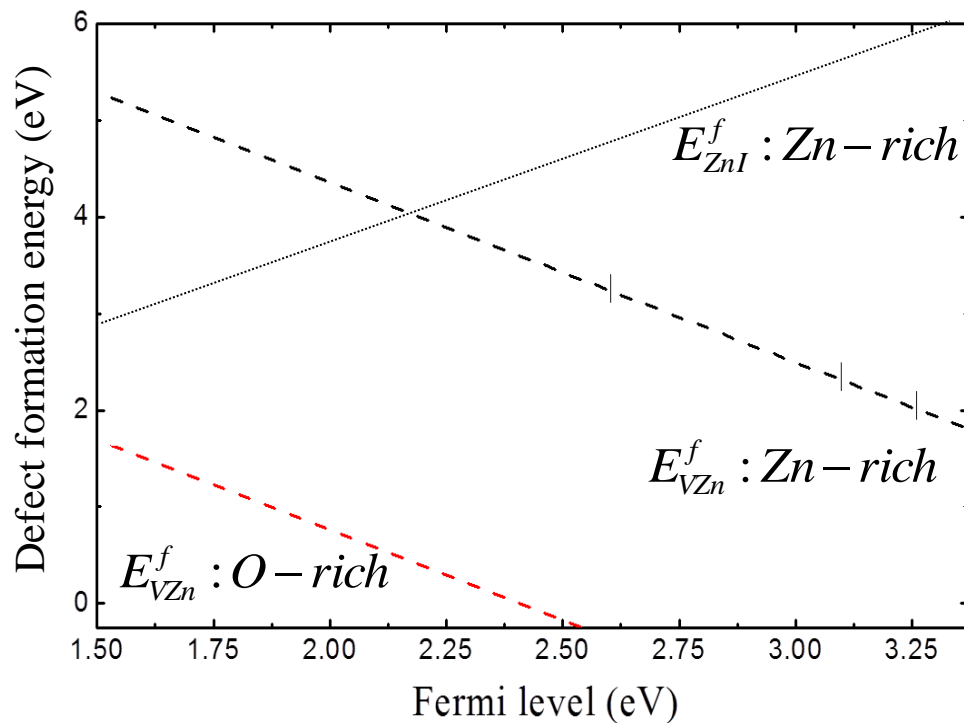
(i) experimentally accessible E_F values are in the upper part of the band gap

(ii) theoretically predicted trends for V_{Zn} and Zn_I formation energies go in opposite directions

(iii) Zn self-diffusion activation energy is a combination of the formation and migration energies of defects mediating the diffusion

Zn self-diffusion revealing V_{Zn} energetics

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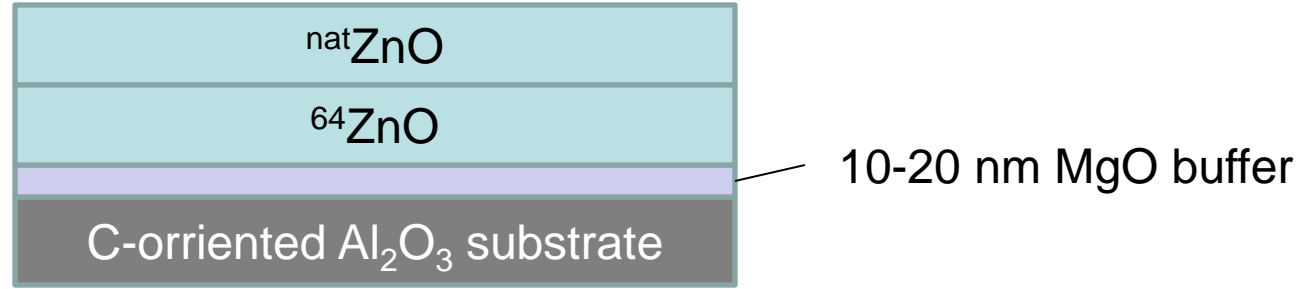
- (i) experimentally accessible E_F values are in the upper part of the band gap
- (ii) theoretically predicted trends for V_{Zn} and Zn_I formation energies go in opposite directions
- (iii) Zn self-diffusion activation energy is a combination of the formation and migration energies of defects mediating the diffusion

Thus, the trend for Zn diffusion activation energy should follow the defect formation energy trends for V_{Zn} or Zn_I assuming the defect migration energy is independent of the Fermi level and the chemical potential.

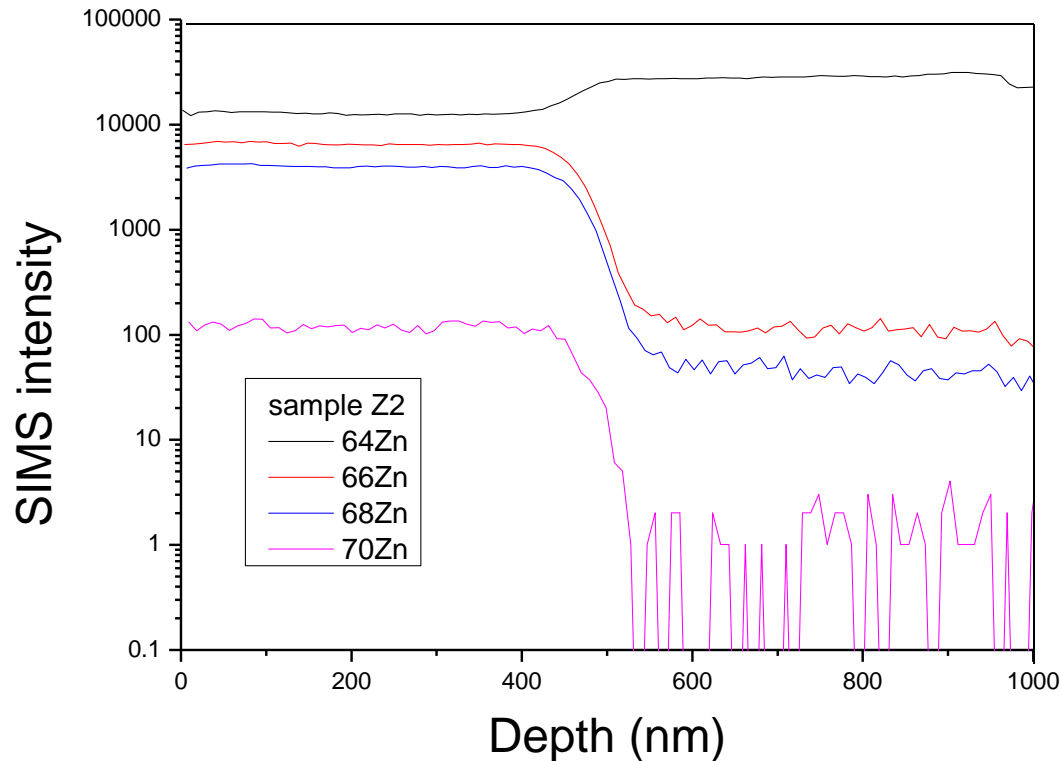
$$D_{Zn}^V = D_0^V e^{-(E_{VZn}^f + E_{VZn}^m)/kT}$$

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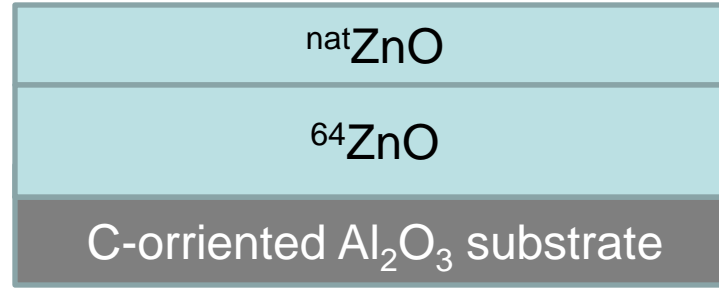
Zn self-diffusion revealing V_{Zn} energetics



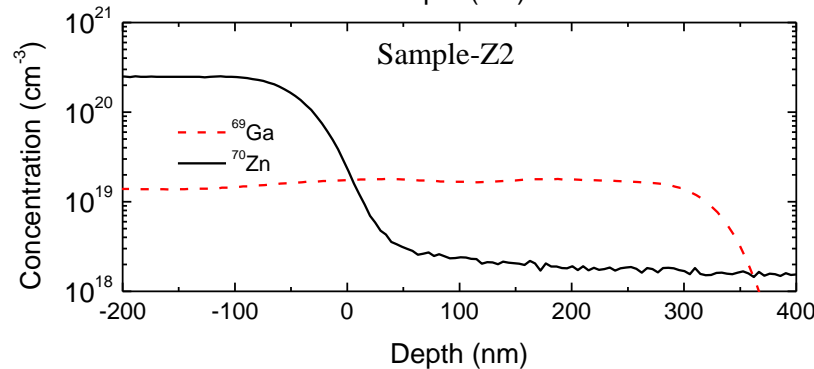
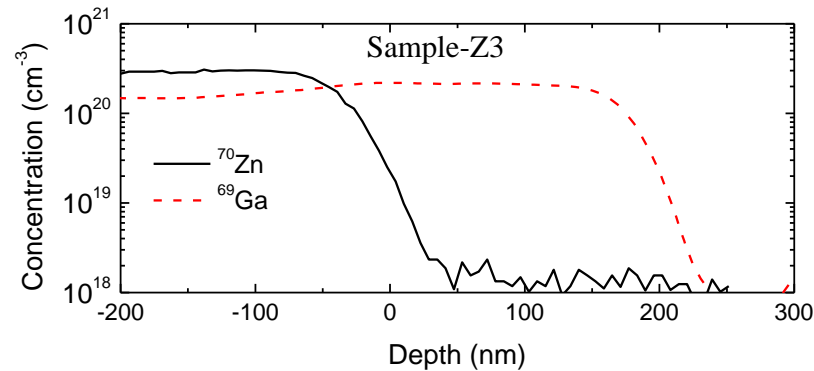
Samples - isotopic $^{nat}\text{ZnO}/^{64}\text{ZnO}$ heterostructures grown by rf-MBE



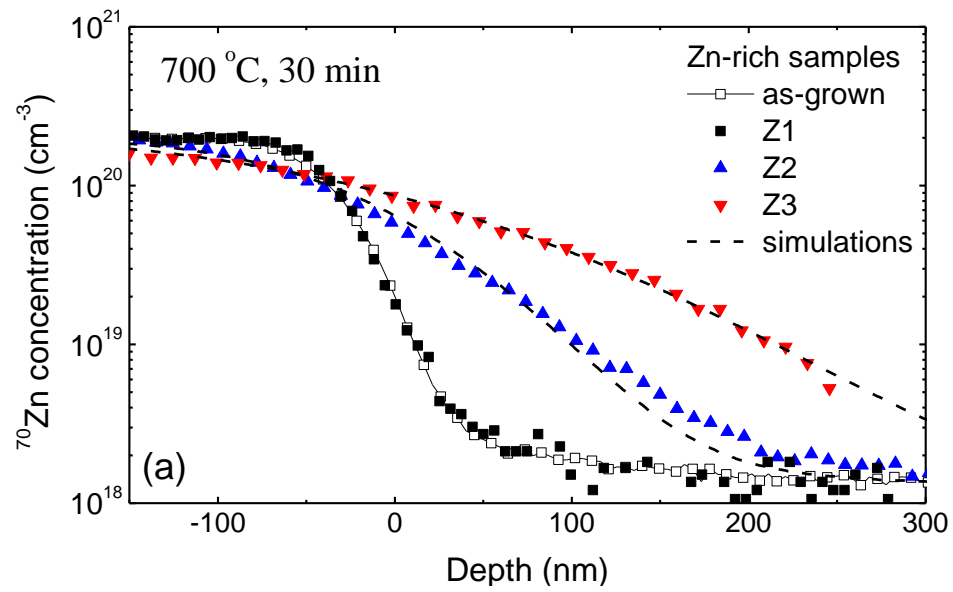
Zn self-diffusion revealing V_{Zn} energetics



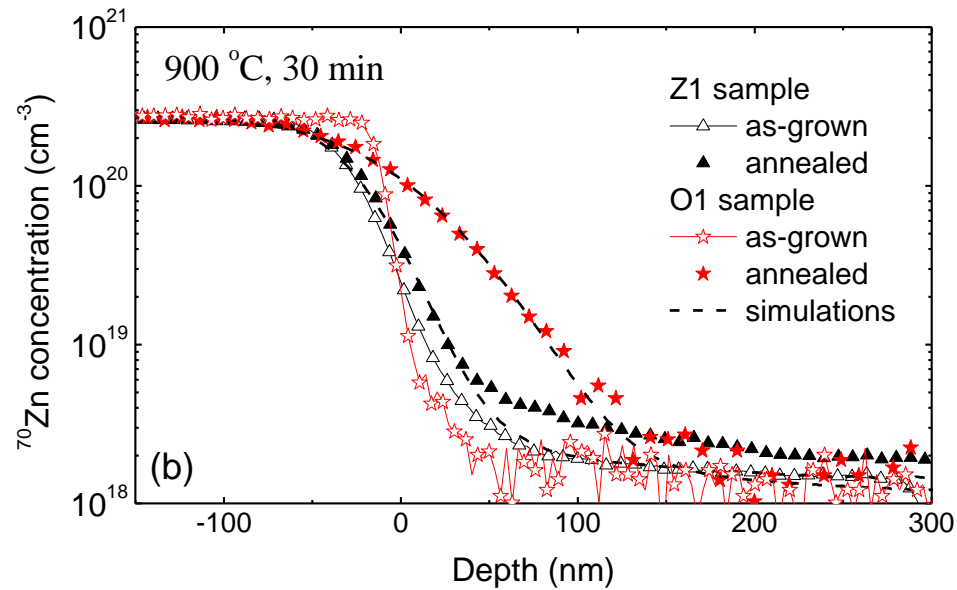
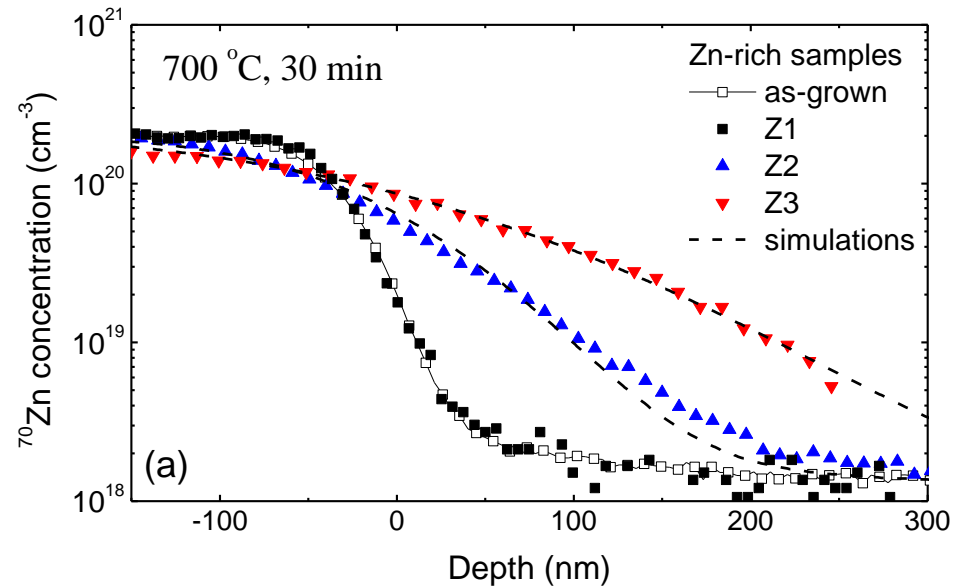
Samples - isotopic $natZnO/^{64}ZnO$ heterostructures grown by rf-MBE



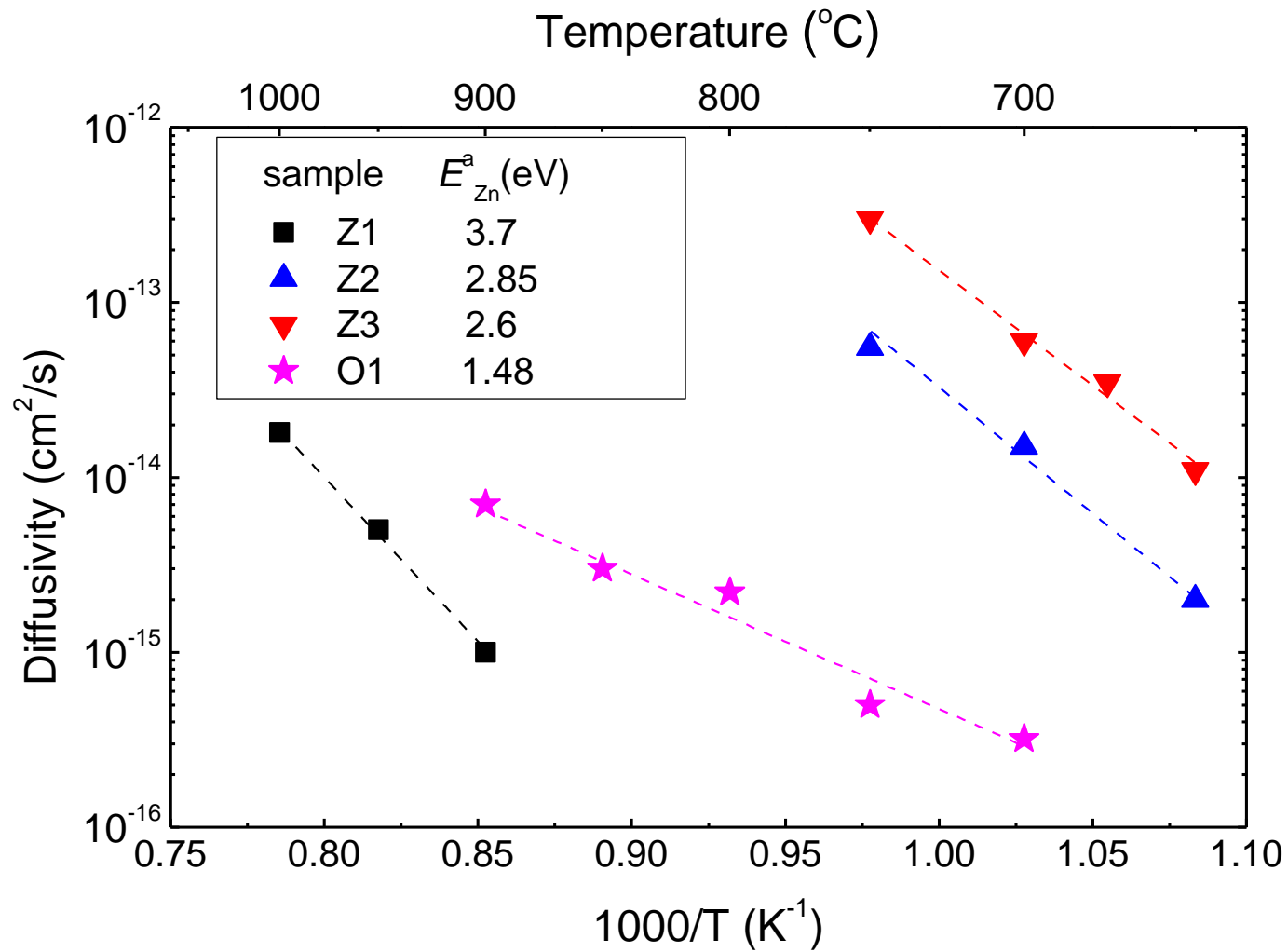
Zn self-diffusion revealing V_{Zn} energetics



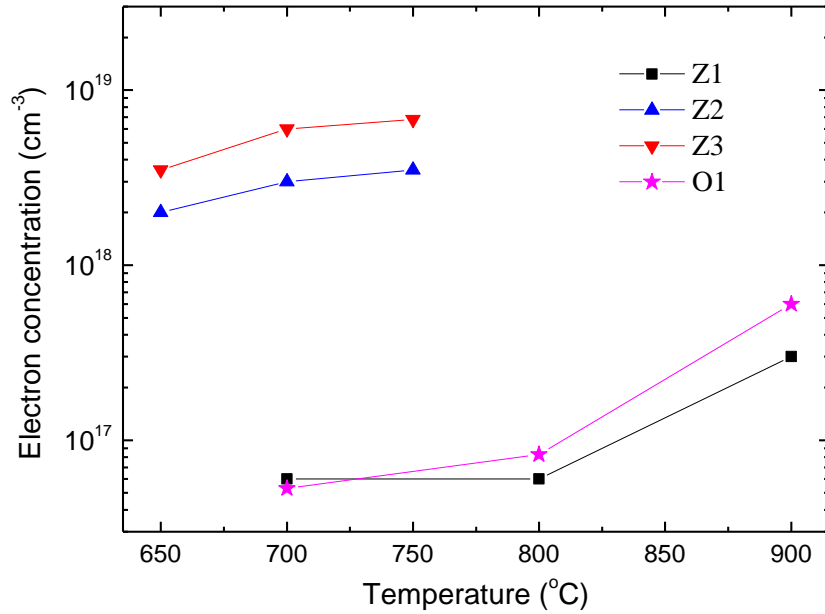
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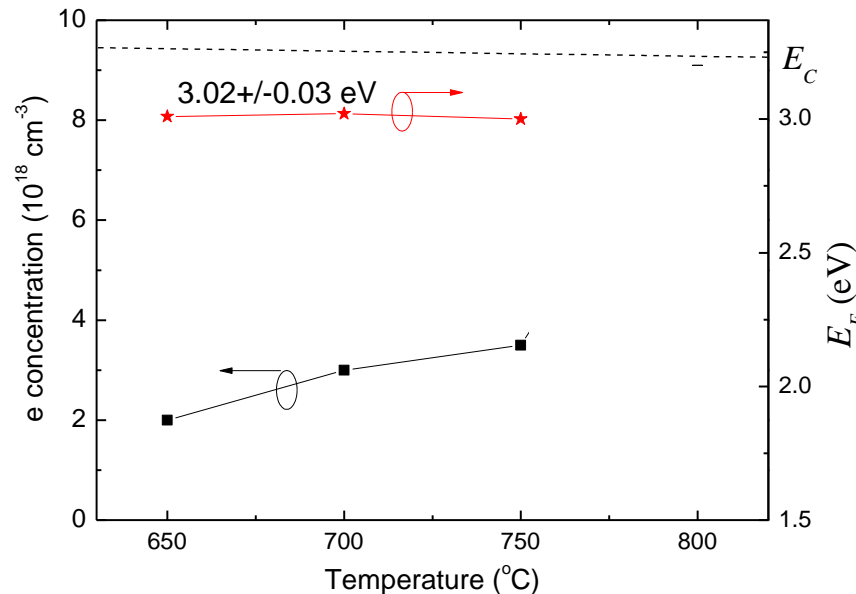
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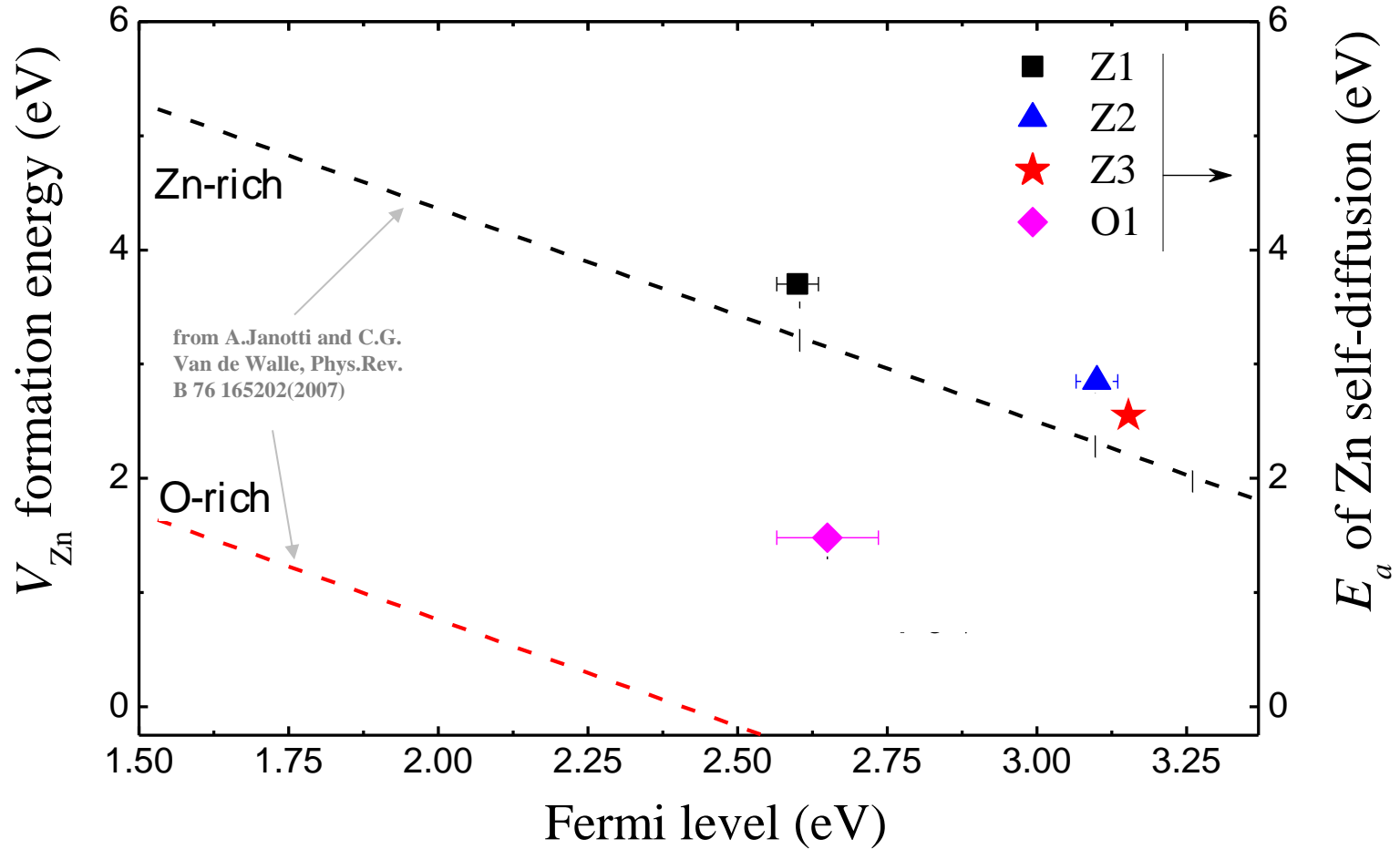
$$E_F = E_F^i + kT \ln \left(\frac{n_c}{n_i} \right),$$

$$n_i = (N_c N_v)^{1/2} \exp \left(-\frac{E_g(T)}{2kT} \right),$$

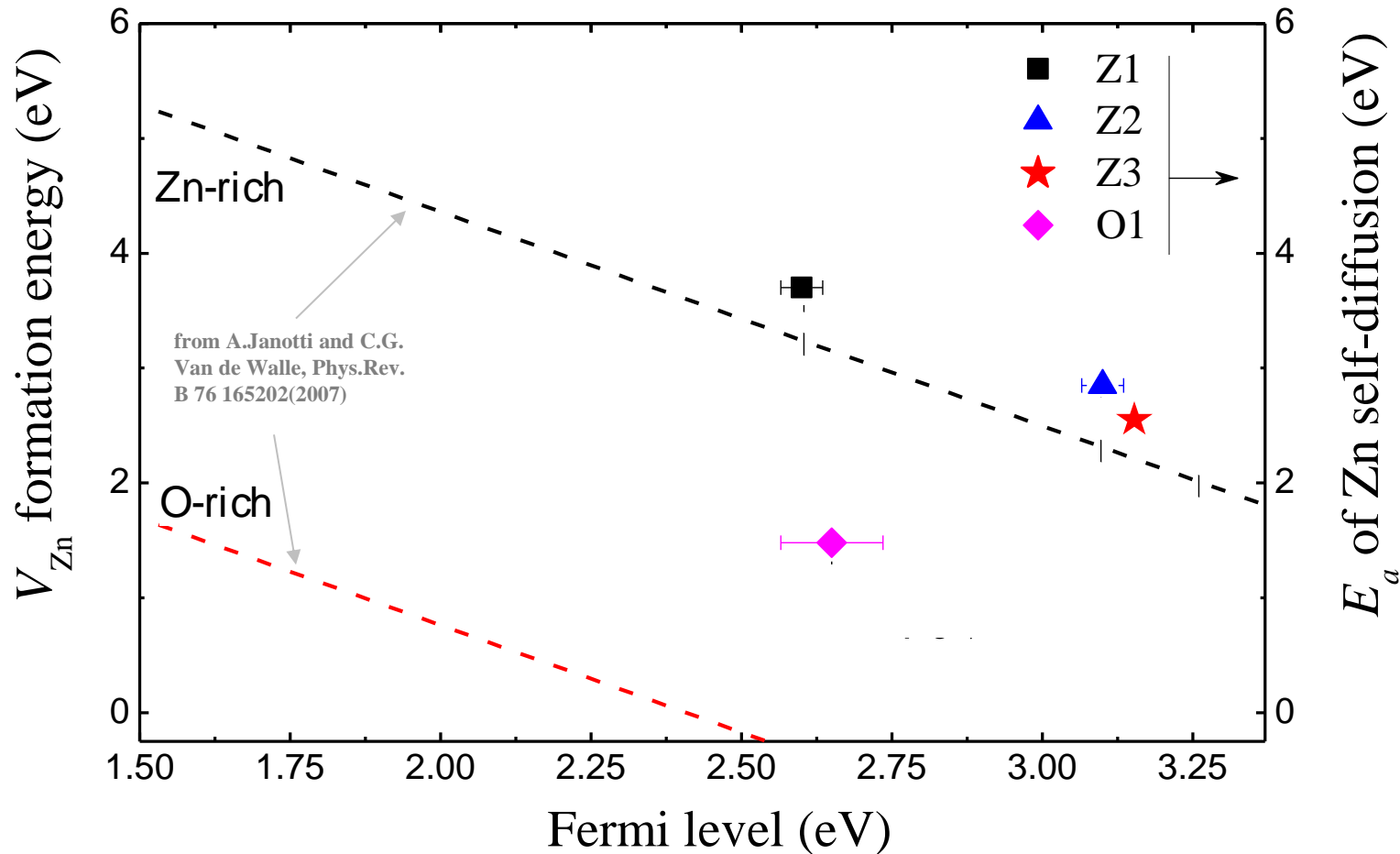
$$N_{c,v} = 2 \left(\frac{2\pi m_{e,h} kT}{h^2} \right)^{3/2},$$



Zn self-diffusion revealing V_{Zn} energetics



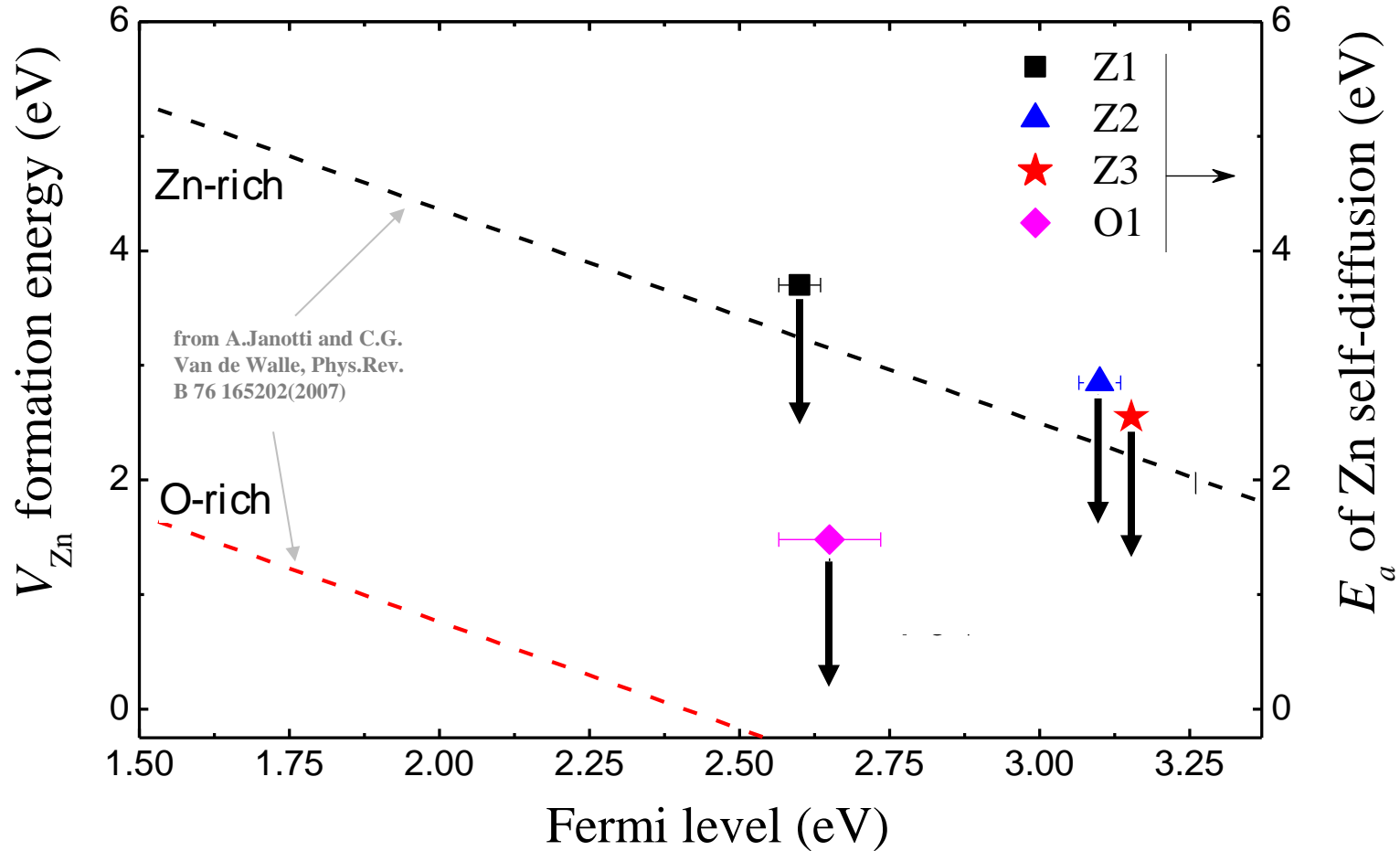
Zn self-diffusion revealing V_{Zn} energetics



E_a values follow the V_{Zn} energy formation trend suggesting Zn to

diffuse in ZnO via vacancy mechanism, i.e $E_a^{Zn} = E_{VZn}^f + E_{VZn}^m$

Zn self-diffusion revealing V_{Zn} energetics



Accounting that $E_a^{Zn} = E_{VZn}^f + E_{VZn}^m$ and the upper limit of the V_{Zn} migration energy can not be higher than the lowest E_a value, we can subtract 1.4 eV to obtain estimates of V_{Zn} formation energies.

Zn self-diffusion revealing V_{Zn} energetics

