

FYS3410 - Vår 2011 (Kondenserte fasers fysikk)

<http://www.uio.no/studier/emner/matnat/fys/FYS3410/index-eng.xml>

Based on Introduction to Solid State Physics by Kittel

Course content

- **Periodic structures, understanding of diffraction experiment and reciprocal lattice**
- **Imperfections in crystals: diffusion, point defects, dislocations**
- **Crystal vibrations: phonon heat capacity and thermal conductivity**
- **Free electron Fermi gas: density of states, Fermi level, and electrical conductivity**
- **Electrons in periodic potential: energy bands theory classification of metals, semiconductors and insulators**
- **Semiconductors: band gap, effective masses, charge carrier distributions, doping, pn-junctions**
- **Metals: Fermi surfaces, temperature dependence of electrical conductivity**

**Andrej Kuznetsov, Dept of Physics and Centre for Material Science and Nanotechnology
Postboks 1048 Blindern, 0316 OSLO
Tel: +47-22852870, e-post: andrej.kuznetsov@fys.uio.no
visiting address: MiNaLab, Gaustadaleen 23b**

FYS3410 lecture schedule and exams: Spring 2011

W/19/1/2011:	Introduction and motivation. Periodicity and lattices	1h
M/24/1/2011:	Index system for crystal planes. Crystal structures	2h
W/26/1/2011:	Reciprocal space, Laue condition and Ewald construction	1h
M/31/1/2011:	Brillouin Zones. Interpretation of a diffraction experiment	2h
W/02/2/2011:	Crystal binding, elastic strain and waves	1h
M/07/2/2011:	Elastic waves in cubic crystals; defects in crystals	2h
W/09/2/2011:	Defects in crystals; case study – vacancies; diffusion	2h
M/14/2/2011:	Crystal vibrations and phonons	2h
W/16/2/2011:	Lattice heat capacity: Dulong-Petit and Einstein models	2h
M/21/2/2011:	Phonon density of states (DOS) and Debye model	2h
W/23/2/2011:	General result for DOS; role of anharmonic interactions	2h
M/28/2/2011:	Thermal conductivity and repetition of crystal vibrations	2h
W/02/3/2011:	no lectures	
M/07/3/2011:	no lectures	
W/09/3/2011:	no lectures	
M/14/3/2011:	Free electron Fermi gas in 1D and 3D – ground state	2h
W/17/3/2011:	Density of states, effect of temperature – FD distribution	1h
M/21/3/2011:	Heat capacity of FEFG	2h
W/23/3/2011:	Repetition	1h
M/28/3/2011:	Mid-term exam	

M/04/4/2011:	Electrical and thermal conductivity in metals	2h
W/06/4/2011:	Bragg reflection of electron waves at the boundary of BZ	2h
M/11/4/2011:	Energy bands, Kronig - Penny model	2h
W/13/4/2011:	Empty lattice approximation; number of orbitals in a band	2h

Påsk uppehåll

W/27/4/2011 no lectures

M/02/5/2011: no lectures

W/04/5/2011: no lectures

M/09/5/2010:	Semiconductors, effective mass method, intrinsic carriers	2h
W/11/4/2010:	Impurity states in semiconductors and carrier statistics	2h
M/16/5/2010:	p-n junctions, Schottky contacts and heterojunctions	2h
W/18/5/2010:	Metals and Fermi surfaces	1h
M/23/5/2010:	Repetition	2h
26-27/5/2010:	Final Exam (sensor:???)	

Lecture 6: Elastic waves in cubic crystals; defects in crystals

- **elastic waves in cubic crystals**
- **defects in crystals**

Lecture 6: Elastic waves in cubic crystals; defects in crystals

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stress $\sigma = \frac{\text{load } W}{\text{area } A}$

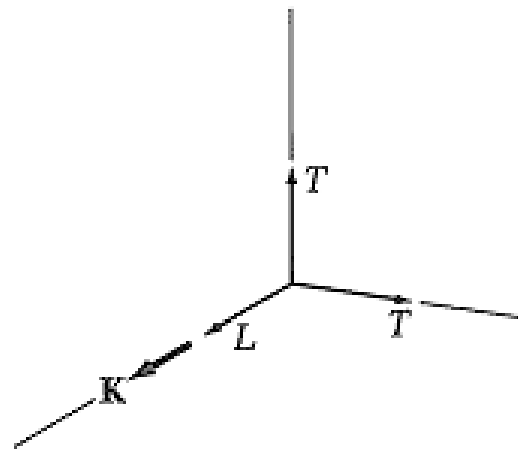
strain $\varepsilon = \frac{\text{increase in length } x}{\text{original length } L}$

$$\varepsilon_{ij} = S_{ij} \cdot \sigma_{ij}$$

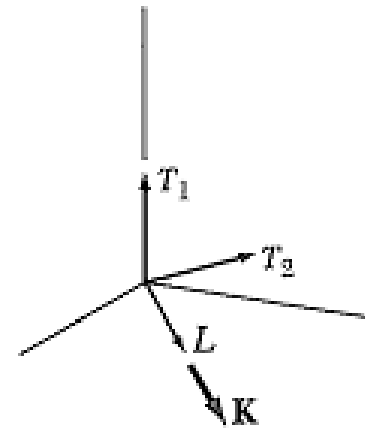
Hooke's law

$$\sigma_{ij} = C_{ij} \cdot \varepsilon_{ij}$$

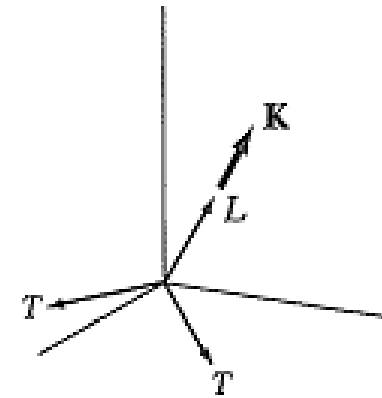
See Eqs 37 and 38 in Kittel, p.77



Wave in [100] direction
 $L : C_{11}$
 $T : C_{44}$



Wave in [110] direction
 $L : \frac{1}{2}(C_{11} + C_{12} + 2C_{44})$
 $T_1 : C_{44}$
 $T_2 : \frac{1}{2}(C_{11} - C_{12})$



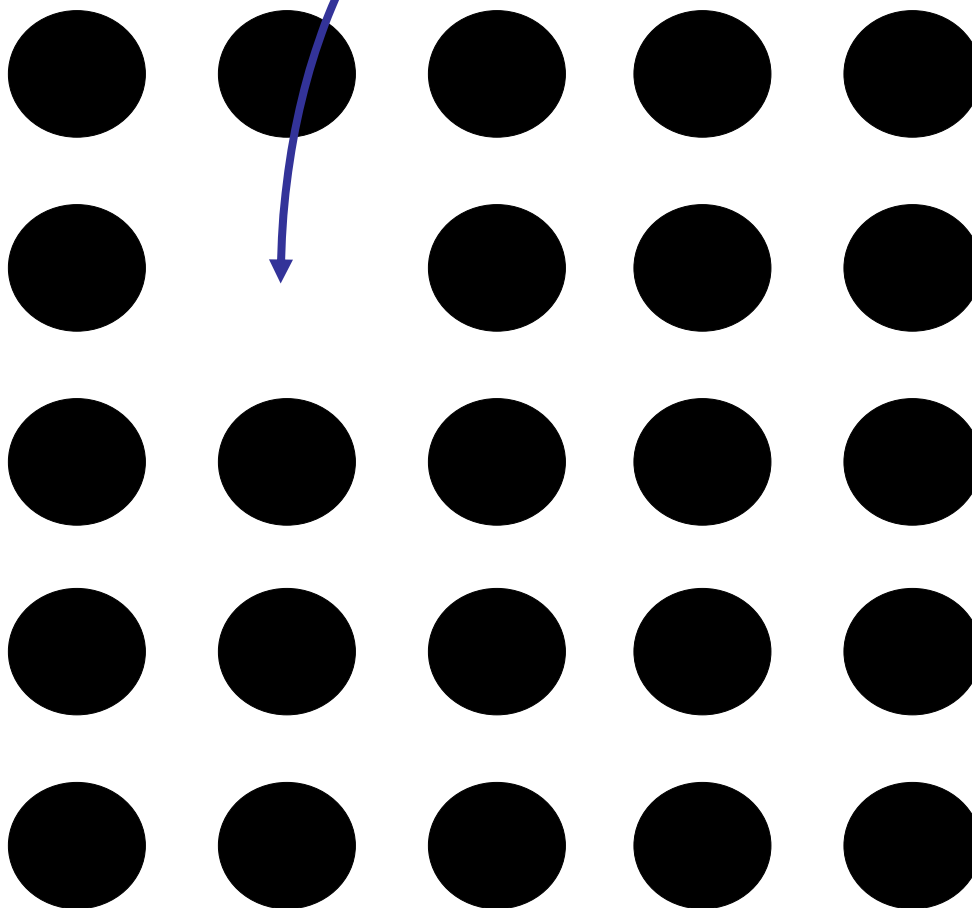
Wave in [111] direction
 $L : \frac{1}{3}(C_{11} + 2C_{12} + 4C_{44})$
 $T : \frac{1}{3}(C_{11} - C_{12} + C_{44})$

Figure 20 Effective elastic constants for the three modes of elastic waves in the principal propagation directions in cubic crystals. The two transverse modes are degenerate for propagation in the [100] and [111] directions.

Lecture 6: Elastic waves in cubic crystals; defects in crystals

- elastic waves in cubic crystals
- **defects in crystals**

Vacancy: A point defect



<i>Defects</i>	<i>Dimensionality</i>	<i>Examples</i>
Point	0	Vacancy
Line	1	Dislocation
Surface	2	Free surface, Grain boundary

Case study: vacancy

Fact

There *may* be vacant sites in a crystal

Surprising Fact

There *must* be a certain fraction of vacant sites in a crystal in *equilibrium*.

Case study: vacancy

- Crystal in equilibrium
- Minimum Gibbs free energy G at constant T and P
- A certain concentration of vacancy lowers the free energy of a crystal

Case study: vacancy

Gibbs free energy G involves two terms:

1. Enthalpy $H = E + PV$

E internal energy

P pressure

V volume

2. Entropy $S = k \ln W$

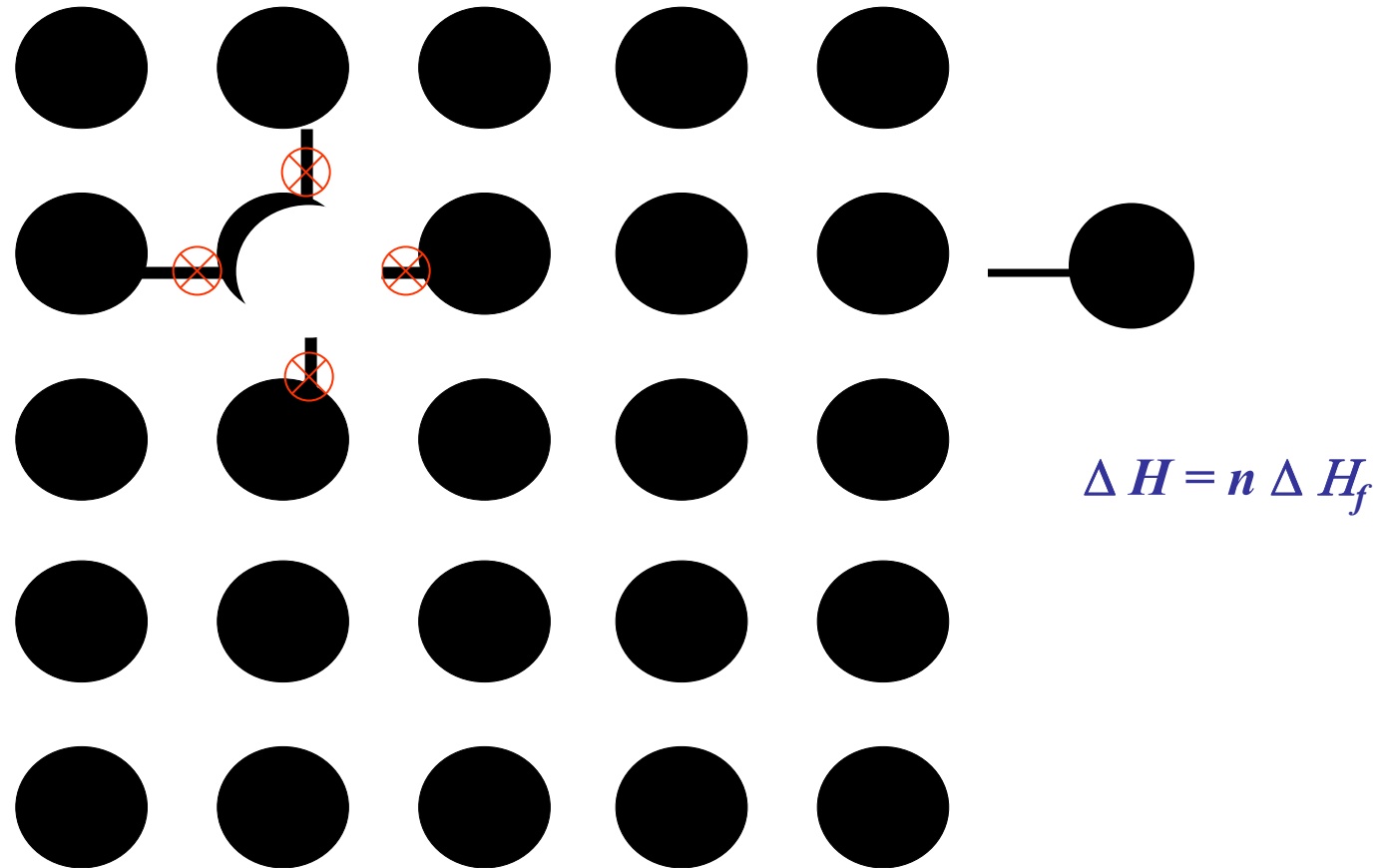
k Boltzmann constant

W number of microstates

$$G = H - TS$$

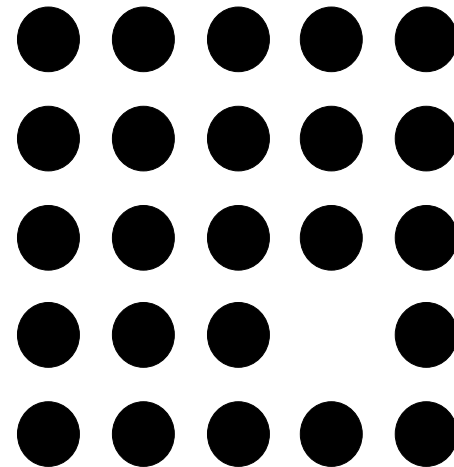
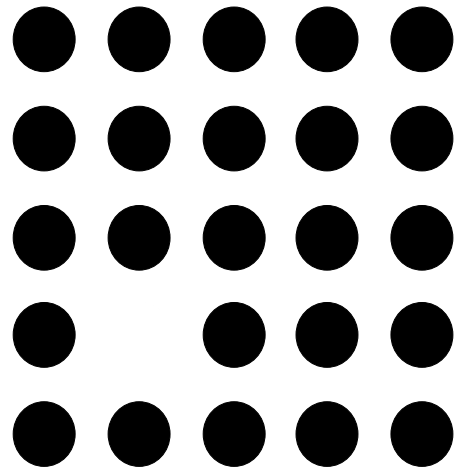
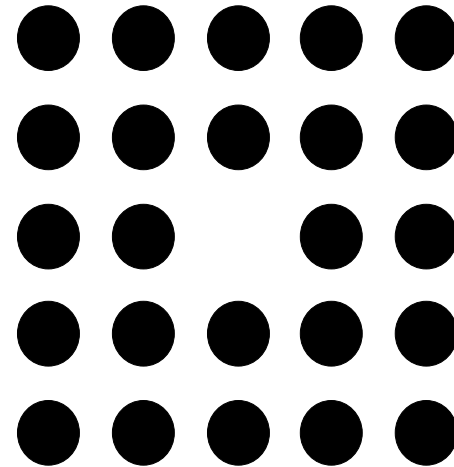
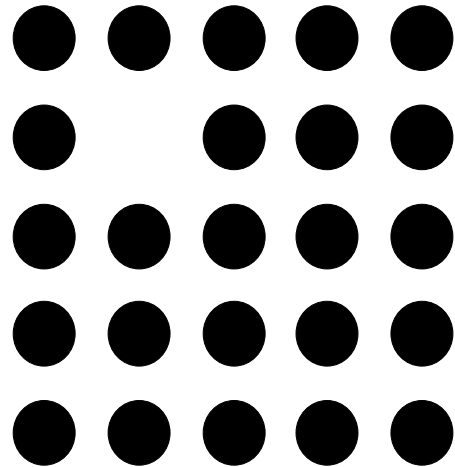
T Absolute temperature

Case study: vacancy



Vacancy increases H of the crystal due to energy required to break bonds

Configurational entropy due to vacancy



Configurational entropy due to vacancy

Number of atoms: N

Number of vacancies: n

Total number of sites: $N+n$

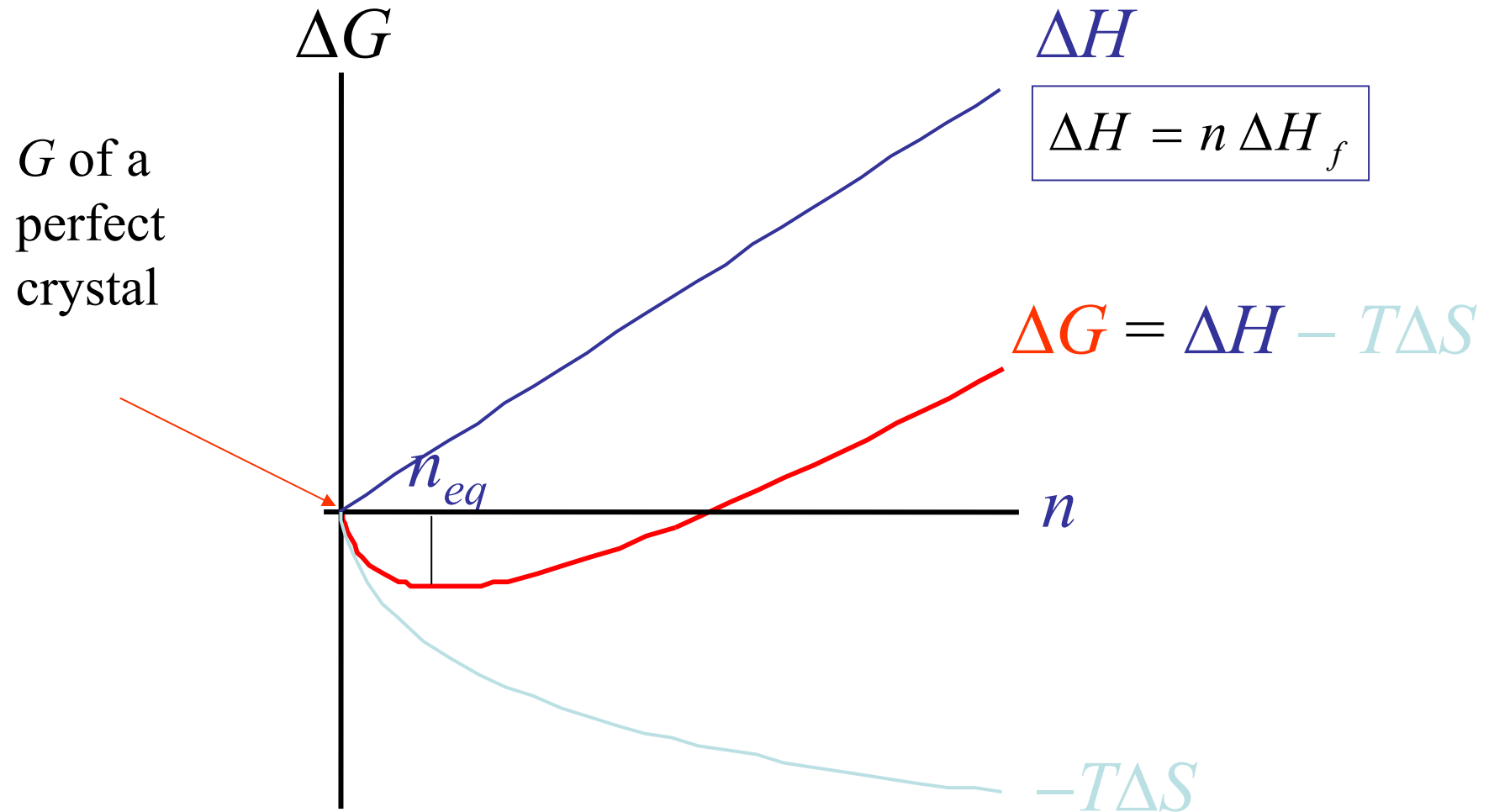
How many distinguished configurations,
so called microstates?

We calculate this explicitly

Configurational entropy due to vacancy

N	$\ln N!$	$N \ln N - N$
1	0	-1
10	15.10	13.03
100	363.74	360.51

Equilibrium concentration of vacancy



Equilibrium concentration of vacancy

$$\left. \frac{\partial \Delta G}{\partial n} \right|_{n=n_{eq}} = 0$$

$$\frac{n_{eq}}{N} = \exp\left(-\frac{\Delta H_f}{kT}\right)$$