FYS3410 - Vår 2010 (Kondenserte fasers fysikk)

Based on Introduction to Solid State Physics by Kittel

Course content

- Periodic structures, understanding of diffraction experiment and reciprocal lattice
- **Crystal binding, elastic strain and waves**
- 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 Nanothechnology
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 2010

|		
M/18/1/2010:	Introduction and motivation. Periodicity and lattices	2h
W/20/1/2010:	Index system for crystal planes. Crystal structures	1h
M/25/1/2010:	Reciprocal space, Laue condition and Ewald construction	2h
W/27/1/2010:	Brillouin Zones. Interpretation of a diffraction experiment	1h
M/01/2/2010:	Crystal binding, elastic strain and waves	2h
W/03/2/2010:	Point defects, case study – vacancies	1h
M/08/2/2010:	Point defects and atomic diffusion	2h
W/10/2/2010:	Diffusion (continuation); dislocations	1h
M/15/2/2010:	Crystal vibrations and phonons	2h
W/17/2/2010:	Crystal vibrations and phonons	1h
M/22/2/2010:	Planck distribution and density of states	2h
W/24/2/2010:	Debye model	1h
M/01/3/2010:	Einstein model and general result for density of states	2h
W/03/3/2010:	Thermal conductivity	1h
M/08/3/2010:	Free electron Fermi gas in 1D and 3D – ground state	2h
W/10/3/2010:	Density of states, effect of temperature – FD distribution	1h
M/15/3/2010:	Heat capacity of FEFG	2h
W/17/3/2010:	Repetition	1h
22/3/2010:	Mid-term exam	

M/14/4/2010:	**Electrical and thermal conductivity in metals**	**2h**
W/12/4/2010:	**Bragg reflection of electron waves at the boundary of BZ**	**1h**
M/19/4/2010:	**Energy bands, Kronig - Penny model**	**2h**
W/21/4/2010:	**Empty lattice approximation; number of orbitals in a band**	**1h**
M/26/4/2010:	**Semiconductors, effective mass method, intrinsic carriers**	**2h**
W/28/4/2010:	**Impurity states in semiconductors and carrier statistics**	**1h**
M/03/5/2010:	**p-n junctions and heterojunctions**	**2h**
W/05/5/2010:	**surface structure, surface states, Schottky contacts**	**2h**
M/10/5/2010:	**no lectures**	
W/12/5/2010:	**no lectures**	
W/19/5/2010:	**Repetition**	**2h**
W26/5/2010:	**Repetition**	**2h**

28/5/2010: Final Exam (sensor: Prof. Arne Nylandsted Larsen at the Århus University, Denmark, http://person.au.dk/en/anl@phys.au.dk)

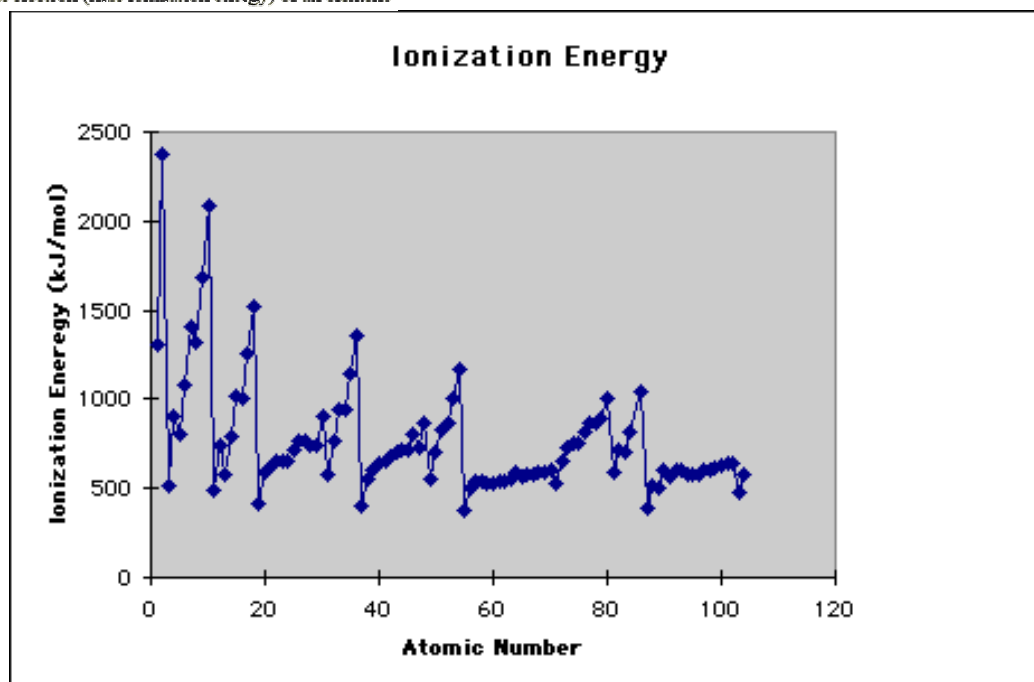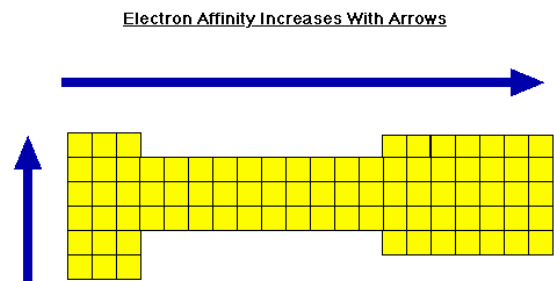**Lecture 5: Crystal binding, elastic strain and waves**

• **ionization and cohesive energies in the context of periodic table;**

• **interaction between two atoms in terms of attraction and repulsion forces;**

• **analysis of elastic strain**

• **elastic waves in cubic crystals**

Lecture 5: Crystal binding, elastic strain and waves

• **ionization and cohesive energies in the context of periodic table;**

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Increase

Decrease

First Ionization Energy
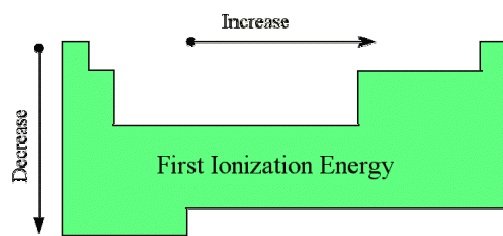
General trends for the energy required to remove the first electron (first ionization energy) of an element

Electron Affinity Increases With Arrows

Ionization Energy

Table 1 Cohesive energies

Energy required to form separated neutral atoms in their ground electronic state from the solid at 0 K at 1 atm. The data were supplied by Prof. Leo Brewer.

Values listed per cell as: kJ/mol · eV/atom · kcal/mol

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Li 158. / 1.63 / 37.7	**Be** 320. / 3.32 / 76.5											**B** 561 / 5.81 / 134	**C** 711 / 7.37 / 170.	**N** 474. / 4.92 / 113.4	**O** 251. / 2.60. / 60.03	**F** 81.0 / 0.84 / 19.37	**Ne** 1.92 / 0.020 / 0.46
Na 107. / 1.113 / 25.67	**Mg** 145. / 1.51 / 34.7											**Al** 327. / 3.39 / 78.1	**Si** 446. / 4.63 / 106.7	**P** 331. / 3.43 / 79.16	**S** 275. / 2.85 / 65.75	**Cl** 135. / 1.40 / 32.2	**Ar** 7.74 / 0.080 / 1.85
K 90.1 / 0.934 / 21.54	**Ca** 178. / 1.84 / 42.5	**Sc** 376 / 3.90 / 89.9	**Ti** 468. / 4.85 / 111.8	**V** 512. / 5.31 / 122.4	**Cr** 395. / 4.10 / 94.5	**Mn** 282. / 2.92 / 67.4	**Fe** 413. / 4.28 / 98.7	**Co** 424. / 4.39 / 101.3	**Ni** 428. / 4.44 / 102.4	**Cu** 336. / 3.49 / 80.4	**Zn** 130 / 1.35 / 31.04	**Ga** 271. / 2.81 / 64.8	**Ge** 372. / 3.85 / 88.8	**As** 285.3 / 2.96 / 68.2	**Se** 237 / 2.46 / 56.7	**Br** 118. / 1.22 / 28.18	**Kr** 11.2 / 0.116 / 2.68
Rb 82.2 / 0.852 / 19.64	**Sr** 166. / 1.72 / 39.7	**Y** 422. / 4.37 / 100.8	**Zr** 603. / 6.25 / 144.2	**Nb** 730. / 7.57 / 174.5	**Mo** 658 / 6.82 / 157.2	**Tc** 661. / 6.85 / 158.	**Ru** 650. / 6.74 / 155.4	**Rh** 554. / 5.75 / 132.5	**Pd** 376. / 3.89 / 89.8	**Ag** 284. / 2.95 / 68.0	**Cd** 112. / 1.16 / 26.73	**In** 243. / 2.52 / 58.1	**Sn** 303. / 3.14 / 72.4	**Sb** 265. / 2.75 / 63.4	**Te** 211 / 2.19 / 50.34	**I** 107. / 1.11 / 25.62	**Xe** 15.9 / 0.16 / 3.80
Cs 77.6 / 0.804 / 18.54	**Ba** 183. / 1.90 / 43.7	**La** 431. / 4.47 / 103.1	**Hf** 621 / 6.44 / 148.4	**Ta** 782. / 8.10 / 186.9	**W** 859. / 8.90 / 205.2	**Re** 775. / 8.03 / 185.2	**Os** 788. / 8.17 / 188.4	**Ir** 670. / 6.94 / 160.1	**Pt** 564. / 5.84 / 134.7	**Au** 368. / 3.81 / 87.96	**Hg** 65. / 0.67 / 15.5	**Tl** 182. / 1.88 / 43.4	**Pb** 196. / 2.03 / 46.78	**Bi** 210. / 2.18 / 50.2	**Po** 144. / 1.50 / 34.5	**At**	**Rn** 19.5 / 0.202 / 4.66
Fr	**Ra** 160. / 1.66 / 38.2	**Ac** 410. / 4.25 / 98.															

Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
417. / 4.32 / 99.7	357. / 3.70 / 85.3	328. / 3.40 / 78.5		206. / 2.14 / 49.3	179. / 1.86 / 42.8	400. / 4.14 / 95.5	391. / 4.05 / 93.4	294. / 3.04 / 70.2	302. / 3.14 / 72.3	317. / 3.29 / 75.8	233. / 2.42 / 55.8	154. / 1.60 / 37.1	428. / 4.43 / 102.2

Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr
598. / 6.20 / 142.9		536. / 5.55 / 128.	456 / 4.73 / 109.	347. / 3.60 / 83.0	264. / 2.73 / 63.	385 / 3.99 / 92.1							

Kcal/mol = 0.0434 eV/molecule   KJ/mol = 0.0104 eV/molecule

Table 2 Melting points, in K.

(After R. H. Lamoreaux)

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Li 453.7	**Be** 1562											**B** 2365	**C**	**N** 63.15	**O** 54.36	**F** 53.48	**Ne** 24.56
Na 371.0	**Mg** 922											**Al** 933.5	**Si** 1687	**P** w 317 / r 863	**S** 388.4	**Cl** 172.2	**Ar** 83.81
K 336.3	**Ca** 1113	**Sc** 1814	**Ti** 1946	**V** 2202	**Cr** 2133	**Mn** 1520	**Fe** 1811	**Co** 1770	**Ni** 1728	**Cu** 1358	**Zn** 692.7	**Ga** 302.9	**Ge** 1211	**As** 1089	**Se** 494	**Br** 265.9	**Kr** 115.8
Rb 312.6	**Sr** 1042	**Y** 1801	**Zr** 2128	**Nb** 2750	**Mo** 2895	**Tc** 2477	**Ru** 2527	**Rh** 2236	**Pd** 1827	**Ag** 1235	**Cd** 594.3	**In** 429.8	**Sn** 505.1	**Sb** 903.9	**Te** 722.7	**I** 386.7	**Xe** 161.4
Cs 301.6	**Ba** 1002	**La** 1194	**Hf** 2504	**Ta** 3293	**W** 3695	**Re** 3459	**Os** 3306	**Ir** 2720	**Pt** 2045	**Au** 1338	**Hg** 234.3	**Tl** 577	**Pb** 600.7	**Bi** 544.6	**Po** 527	**At**	**Rn**
Fr	**Ra** 973	**Ac** 1324															

Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
1072	1205	1290		1346	1091	1587	1632	1684	1745	1797	1820	1098	1938

Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lw
2031	1848	1406	910	913	1449	1613	1562						

At atmospheric pressure carbon has no melting point as its triple point is at
10.8 ± 0.2 MPa and 4600 ± 300 K, so it sublimates at about 3900 K
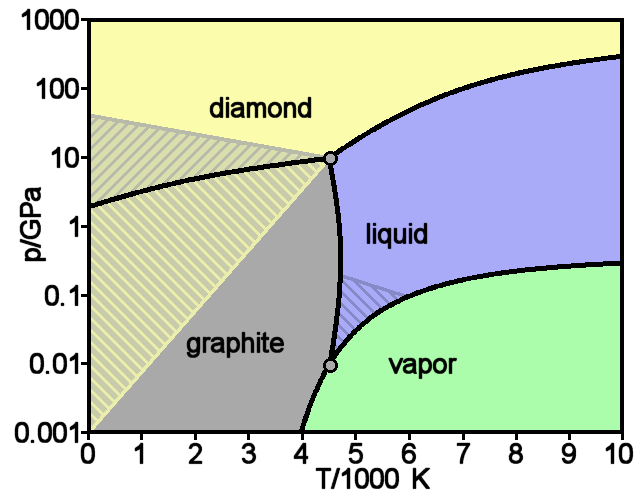
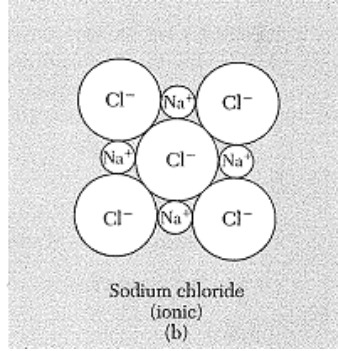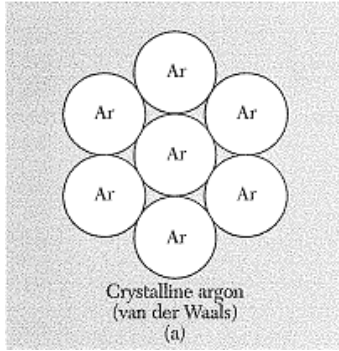101.325 kPa is "one standard atmosphere" and **1 Pa** = 1 N/m2

$$1\ \text{J} = 1\ \text{N} \cdot \text{m} = \left(\frac{\text{kg} \cdot \text{m}}{\text{s}^2}\right) \cdot \text{m} = \frac{\text{kg} \cdot \text{m}^2}{\text{s}^2} = \text{Pa} \cdot \text{m}^3 = 1\ \text{W} \cdot \text{s}$$

1 eV = 1.602176487×10−19 Joule

Lecture 5: Crystal binding, elastic strain and waves

• ionization and cohesive energies in the context of periodic table;

• **interaction between two atoms in terms of attraction and repulsion forces;**

• analysis of elastic strain

• elastic waves in cubic crystals

Crystalline argon (van der Waals) (a)

Sodium chloride (ionic) (b)

Sodium (metallic) (c)

Diamond (covalent) (d)

Cohesive energy = energy required to break up crystal into neutral free atoms.

Lattice energy (ionic crystals) = energy required to break up crystal into free ions.
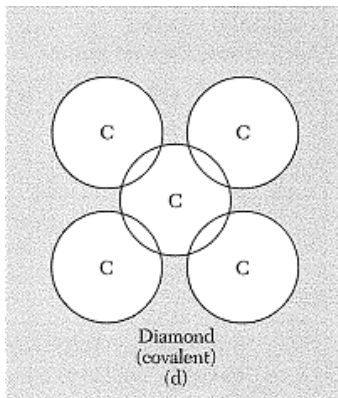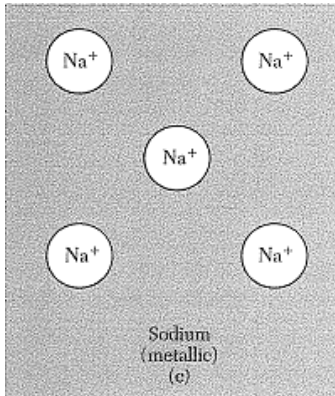
◎ The atoms of the inert gasses attract each other via the so-called Van Der Waals interaction (dipole-dipole interaction)

◎ The unperturbed Hamiltonian of the system is the one of two independent oscillators and is given by:

$$H_0 = \frac{p_1^2}{2m} + \frac{1}{2}cx_1^2 + \frac{p_2^2}{2m} + \frac{1}{2}cx_2^2$$

◎ The interaction energy of the oscillators is given by:

$$H_1 = \frac{1}{4\pi\varepsilon}\left[\frac{e^2}{R} + \frac{e^2}{R+x_2-x_1} - \frac{e^2}{R+x_2} - \frac{e^2}{R-x_1}\right] \approx -2\frac{e^2 x_1 x_2}{4\pi\varepsilon R^3}$$
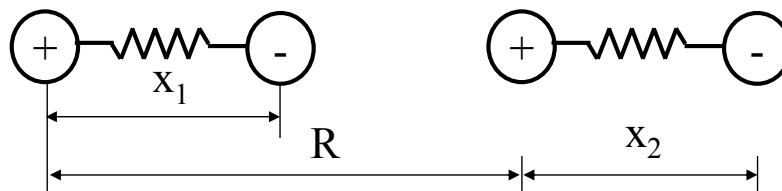
- ◎ Besides the Van der Waals interaction, when two atoms are brought together, their charge distribution begins to overlap, giving rise to the exchange interaction due to the Pauli exclusion principle.

- ◎ Since this interaction is difficult to be evaluated from first principles, it is usually parametrized with a term that goes as 1/R12, which then when added to the Van der Waals term gives rise to the famous Lennard-Jones potential that is of the following form:

$$U(R) = 4\varepsilon \left[\left(\frac{\sigma}{R} \right)^{12} - \left(\frac{\sigma}{R} \right)^{6} \right]$$

1. One first re-writes the Lennard-Jones potential as a sum of all pairs of atoms in the crystal as:

$$U_{TOT}(R) = \frac{1}{2} N(4\varepsilon) \left[\sum_{j} \left(\frac{\sigma}{p_{ij} R} \right)^{12} - \sum_{j} \left(\frac{\sigma}{p_{ij} R} \right)^{6} \right]$$

where $p_{ij} R$ is the distance between the reference atom i and any other atom j. For FCC structure with 12 nearest neighbors, we have:

$$\sum_{j} \left(\frac{1}{p_{ij}} \right)^{12} = 12.13188, \quad \sum_{j} \left(\frac{1}{p_{ij}} \right)^{6} = 14.45392$$

2. The condition that the net force on the atom is zero then gives $R_0/s = 1.09$, and the cohesive energy is:

$$U_{TOT}(R) = -2.15(4N\varepsilon)$$

Crystals of Inert Gases

Table 4 Properties of inert gas crystals

(Extrapolated to 0 K and zero pressure)

	Nearest-neighbor distance, in Å	Experimental cohesive energy		Melting point, K	Ionization potential of free atom, eV	Parameters in Lennard-Jones potential, Eq. 10	
		kJ/mol	eV/atom			ϵ, in 10^{-16} erg	σ, in Å
He	(liquid at zero pressure)				24.58	14	2.56
Ne	3.13	1.88	0.02	24.56	21.56	50	2.74
Ar	3.76	7.74	0.080	83.81	15.76	167	3.40
Kr	4.01	11.2	0.116	115.8	14.00	225	3.65
Xe	4.35	16.0	0.17	161.4	12.13	320	3.98

Atoms:
- high ionization energy
- outermost shell filled
- charge distribution spherical

Crystal:
- transparent insulators
- weakly bonded
- low melting point
- closed packed (fcc, except He^3 & He^4).

Covalent Crystals

H_2
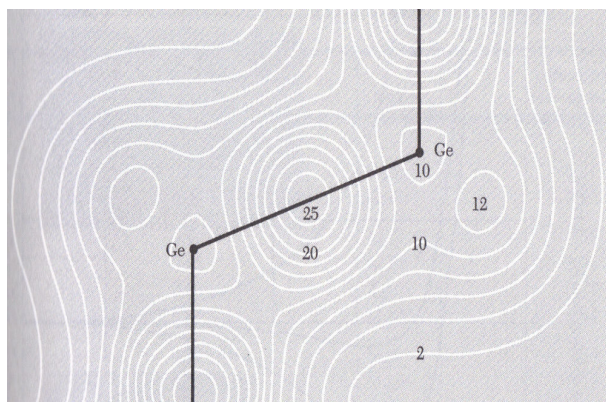
- Electron pair localized midway of bond.
- Tetrahedral: diamond, zinc-blende structures.
- Low filling: 0.34 vs 0.74 for closed-packed.
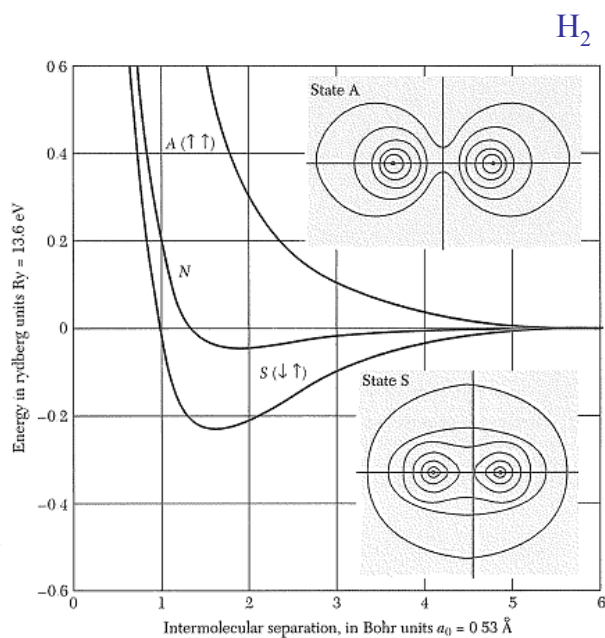
Pauli exclusion →
exchange interaction
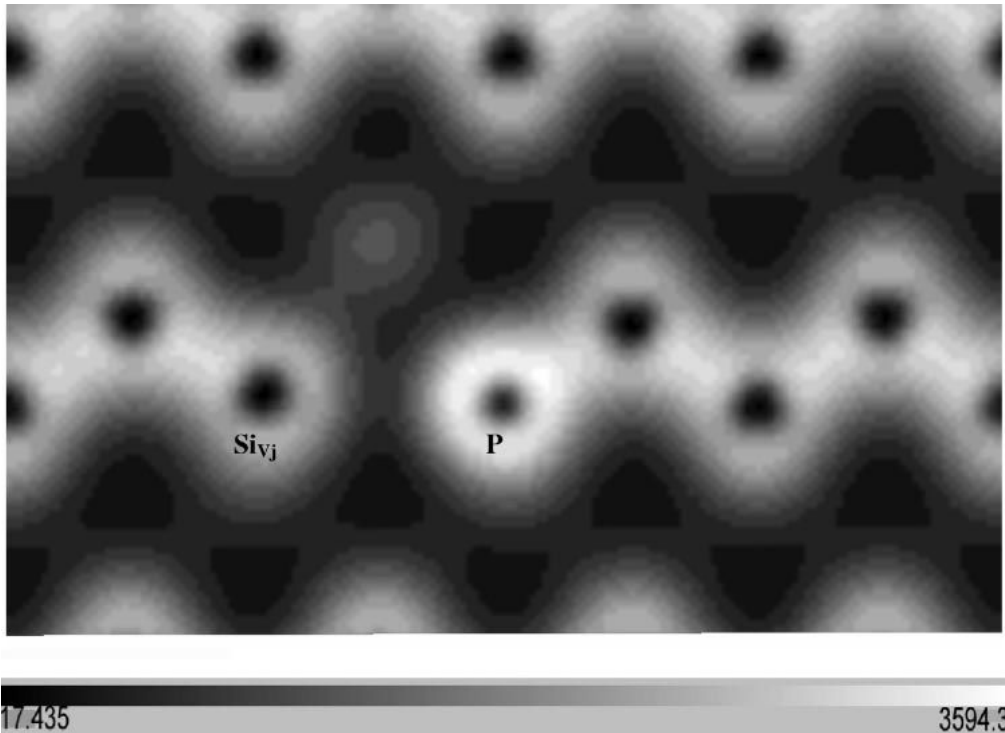
FIG. 4. Electron localization function map for the (110) plane, containing the phosphorus atom and vacancy for the case of the negatively charged PV complex
(PHYSICAL REVIEW B **70**, 115204 (2004))

Lecture 5: Crystal binding, elastic strain and waves

• ionization and cohesive energies in the context of periodic table;

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• **analysis of elastic strain**

• elastic waves in cubic crystals

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

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

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

Hooke's law

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

See Eqs 37 and 38 in Kittel, p.77

Is there a good reason to introduce complications with so many different indexes as in p.73-80? Yes it is, becase, for example elastic waves in crystals often propagate in different directions, specifically can be longitudinal or transverse (share) waves

Elastic strain (deformation)

1. Initial

2. Small load — bonds stretch

δ

F

3. Unload — return to initial

Elastic means reversible!

F — Linear-elastic

Non-Linear-elastic

δ

Plastic deformation

1. Initial

2. Small load

bonds stretch & planes shear

3. Unload

planes still sheared

δ**elastic + plastic**

δ**plastic**

F

Plastic means permanent!

F

linear elastic

linear elastic

δ

δ**plastic**

Elastic/plastic deformation

σ (ksi)

60 σ_U

40 σ_Y

20

Rupture

σ_B

Yield | Strain-hardening | Necking

0.0012   0.02   0.2   0.25

ϵ

(a) Low-carbon steel

σ (ksi)

60 σ_U

40 σ_Y

20

Rupture

σ_B

0.004   0.2

ϵ

(b) Aluminum alloy

Elastic/plastic deformation

Quenched, tempered
alloy steel (A709)

High-strength, low-alloy
steel (A992)

Carbon steel (A36)

Pure iron

- Below the yield stress

$$\sigma = E\varepsilon$$

E = Youngs Modulus or
Modulus of Elasticity

- Strength is affected by alloying, heat treating, and manufacturing process but stiffness (Modulus of Elasticity) is not.

How is strain applied to the electronic chips?
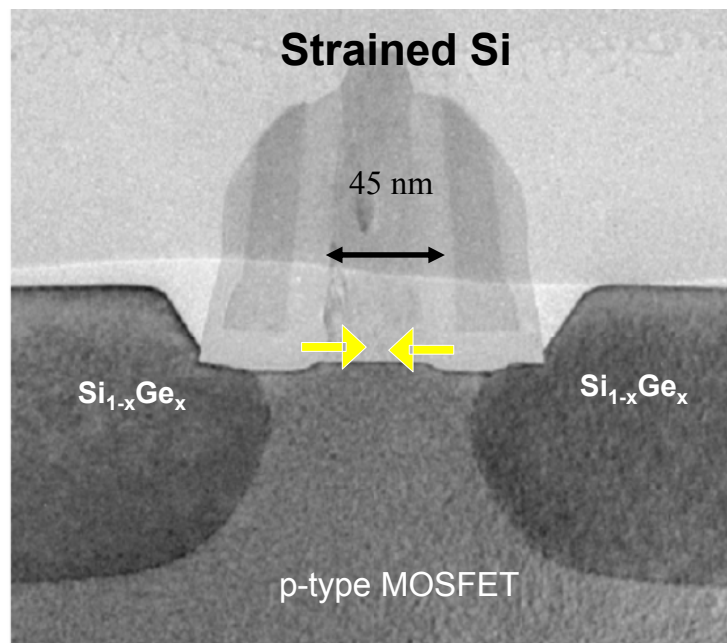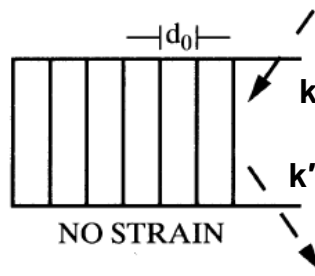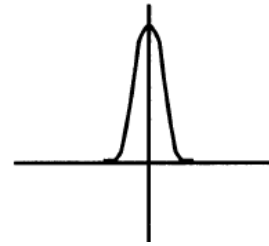
**Strained Si**

45 nm

$Si_{1-x}Ge_x$

$Si_{1-x}Ge_x$

p-type MOSFET

Evolution of x-ray diffraction

CRYSTAL LATTICE

DIFFRACTION LINE

$-|d_0|-$

k

k'

NO STRAIN

Evolution of x-ray diffraction

INCIDENT

2θ

k

K

$-k_o$

CRYSTAL LATTICE

DIFFRACTION LINE

$-|d_0|-$

k

k'

NO STRAIN

2θ

Evolution of x-ray diffraction

CRYSTAL LATTICE

DIFFRACTION LINE

$|d_0|$

k

k'

NO STRAIN

2θ

UNIFORM STRAIN

INCIDENT

2θ

$-k_o$

k

K

Evolution of x-ray diffraction

CRYSTAL LATTICE

DIFFRACTION LINE

$|d_0|$

k

k'

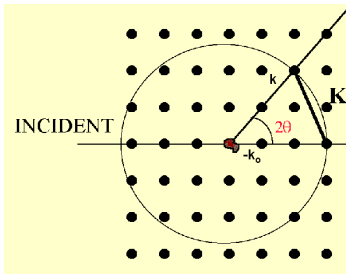NO STRAIN

2θ

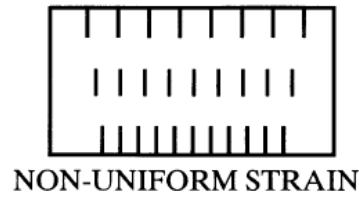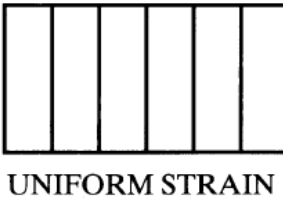UNIFORM STRAIN
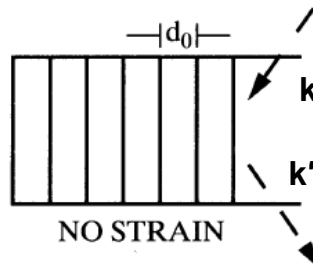
2θ

INCIDENT

2θ

$-k_o$

k

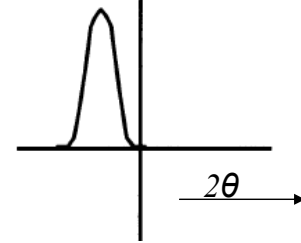**K**

$$n\lambda = 2d\sin\theta$$

Evolution of x-ray diffraction

$$n\lambda = 2d \sin\theta$$

CRYSTAL LATTICE

DIFFRACTION LINE

$|d_0|$

k

k'

NO STRAIN

2θ

UNIFORM STRAIN
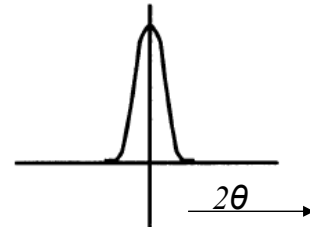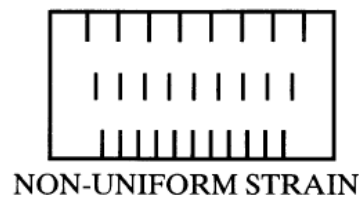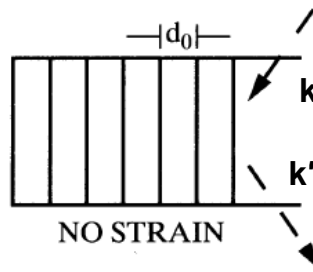
2θ
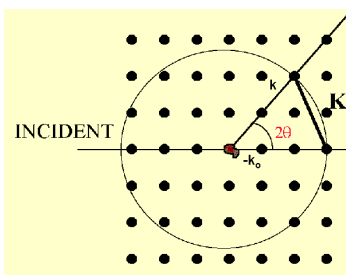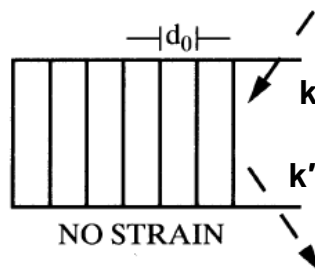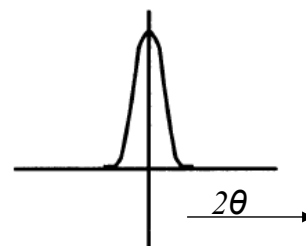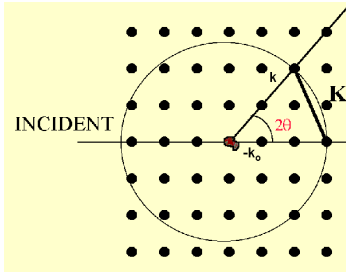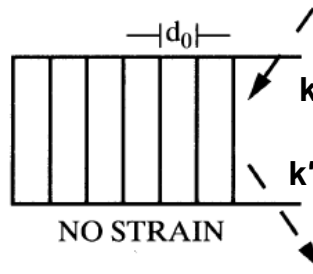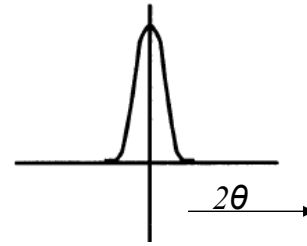
NON-UNIFORM STRAIN

Evolution of x-ray diffraction
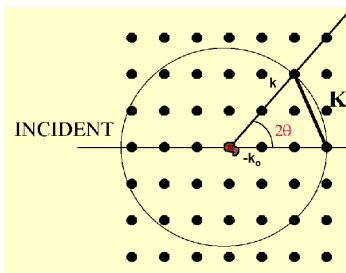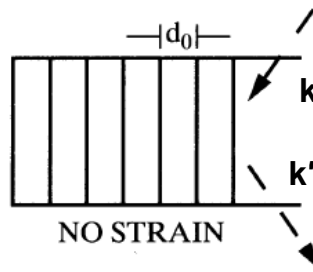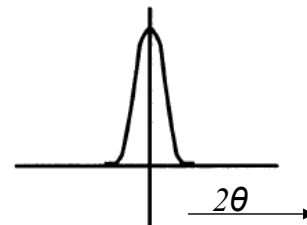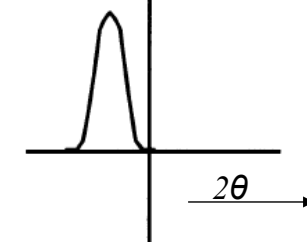
$$n\lambda = 2d \sin\theta$$

CRYSTAL LATTICE

DIFFRACTION LINE

$|d_0|$

k

k'

NO STRAIN

2θ

UNIFORM STRAIN

2θ

NON-UNIFORM STRAIN

2θ
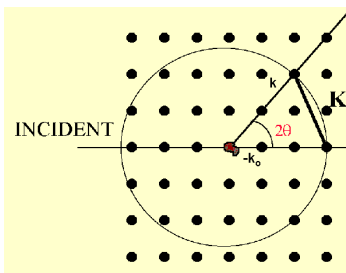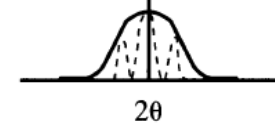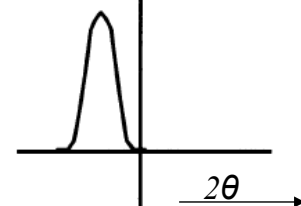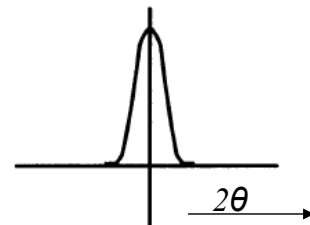
Lecture 5: Crystal binding, elastic strain and waves

• ionization and cohesive energies in the context of periodic table;

• interaction between two atoms in terms of attraction and repulsion forces;

• analysis of elastic strain

• elastic waves in cubic crystals

Elastic Waves in Cubic Crystals

Newton's 2nd law:
$$\rho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial \sigma_{ik}}{\partial x_k}$$

$$\sigma_{ik} = C_{ikjl}\, u_{jl} \qquad \rightarrow \qquad \rho \frac{\partial^2 u_i}{\partial t^2} = C_{ikjl} \frac{\partial u_{jl}}{\partial x_k} = \frac{1}{2} C_{ikjl} \left(\frac{\partial^2 u_l}{\partial x_k \partial x_j} + \frac{\partial^2 u_j}{\partial x_k \partial x_l} \right) = C_{ikjl} \frac{\partial^2 u_l}{\partial x_k \partial x_j}$$

$$\rho \frac{\partial^2 u_1}{\partial t^2} = C_{1111} \frac{\partial^2 u_1}{\partial x_1^2} + C_{1122} \frac{\partial^2 u_2}{\partial x_1 \partial x_2} + C_{1133} \frac{\partial^2 u_3}{\partial x_1 \partial x_3} + C_{1212} \frac{\partial^2 u_2}{\partial x_2 \partial x_1} + C_{1221} \frac{\partial^2 u_1}{\partial x_2^2} + C_{1313} \frac{\partial^2 u_3}{\partial x_3 \partial x_1} + C_{1331} \frac{\partial^2 u_1}{\partial x_3^2}$$

$$= C_{1111} \frac{\partial^2 u_1}{\partial x_1^2} + C_{1122} \left(\frac{\partial^2 u_2}{\partial x_1 \partial x_2} + \frac{\partial^2 u_3}{\partial x_1 \partial x_3} \right) + C_{1212} \left(\frac{\partial^2 u_2}{\partial x_2 \partial x_1} + \frac{\partial^2 u_1}{\partial x_2^2} + \frac{\partial^2 u_3}{\partial x_3 \partial x_1} + \frac{\partial^2 u_1}{\partial x_3^2} \right)$$

$$\therefore \qquad \rho \frac{\partial^2 u_1}{\partial t^2} = C_{11} \frac{\partial^2 u_1}{\partial x_1^2} + \left(C_{12} + C_{44} \right) \left(\frac{\partial^2 u_2}{\partial x_1 \partial x_2} + \frac{\partial^2 u_3}{\partial x_1 \partial x_3} \right) + C_{44} \left(\frac{\partial^2 u_1}{\partial x_2^2} + \frac{\partial^2 u_1}{\partial x_3^2} \right)$$

Similarly
$$\rho \frac{\partial^2 u_2}{\partial t^2} = C_{11} \frac{\partial^2 u_2}{\partial x_2^2} + \left(C_{12} + C_{44} \right) \left(\frac{\partial^2 u_3}{\partial x_2 \partial x_3} + \frac{\partial^2 u_1}{\partial x_2 \partial x_1} \right) + C_{44} \left(\frac{\partial^2 u_2}{\partial x_1^2} + \frac{\partial^2 u_2}{\partial x_3^2} \right)$$

$$\rho \frac{\partial^2 u_3}{\partial t^2} = C_{11} \frac{\partial^2 u_3}{\partial x_3^2} + \left(C_{12} + C_{44} \right) \left(\frac{\partial^2 u_2}{\partial x_3 \partial x_2} + \frac{\partial^2 u_1}{\partial x_3 \partial x_1} \right) + C_{44} \left(\frac{\partial^2 u_3}{\partial x_2^2} + \frac{\partial^2 u_3}{\partial x_1^2} \right)$$

Dispersion Equation

$$\rho \frac{\partial^2 u_i}{\partial t^2} = C_{ikjl} \frac{\partial^2 u_l}{\partial x_k \partial x_j}$$

$$u_i = u_{0i} \, e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)} \qquad \rightarrow \qquad \omega^2 \rho \, u_{0i} = C_{ikjl} \, k_k \, k_j \, u_{0l}$$

$$\left(\omega^2 \rho \, \delta_{il} - C_{ikjl} \, k_k \, k_j \right) u_{0l} = 0$$

$$\left| \omega^2 \rho \, \delta_{il} - C_{ikjl} \, k_k \, k_j \right| = 0 \qquad \text{dispersion equation}$$

$$\left| \omega^2 \rho \, I - \mathbf{C}(\mathbf{k}) \right| = 0 \qquad\qquad C_{ij}(\mathbf{k}) = C_{imnj} \, k_m \, k_n$$

Waves in the [100] direction

$$\left| \omega^2 \rho \, I - \mathbf{C}(\mathbf{k}) \right| = 0 \qquad\qquad C_{ij}(\mathbf{k}) = C_{imnj} \, k_m \, k_n$$

$$\mathbf{k} = k(1,0,0) \qquad \rightarrow \qquad C_{ij}(\mathbf{k}) = C_{i11j} k^2$$

$$\mathbf{C}(\mathbf{k}) = k^2 \begin{pmatrix} C_{1111} & 0 & 0 \\ 0 & C_{2112} & 0 \\ 0 & 0 & C_{3113} \end{pmatrix} = k^2 \begin{pmatrix} C_{11} & 0 & 0 \\ 0 & C_{44} & 0 \\ 0 & 0 & C_{44} \end{pmatrix}$$

$$\omega_L = \sqrt{\frac{C_{11}}{\rho}} \, k \qquad \mathbf{u}_0 = (1,0,0) \qquad \text{Longitudinal}$$

$$\omega_T = \sqrt{\frac{C_{44}}{\rho}} \, k \qquad \begin{aligned} \mathbf{u}_0 &= (0,1,0) \\[4pt] \mathbf{u}_0 &= (0,0,1) \end{aligned} \qquad \text{Transverse, degenerate}$$

Waves in the [110] direction

$$\left| \omega^2 \rho\, I - \mathbf{C(k)} \right| = 0 \qquad\qquad \mathbf{C}_{ij}(\mathbf{k}) = C_{imnj}\, k_m\, k_n$$
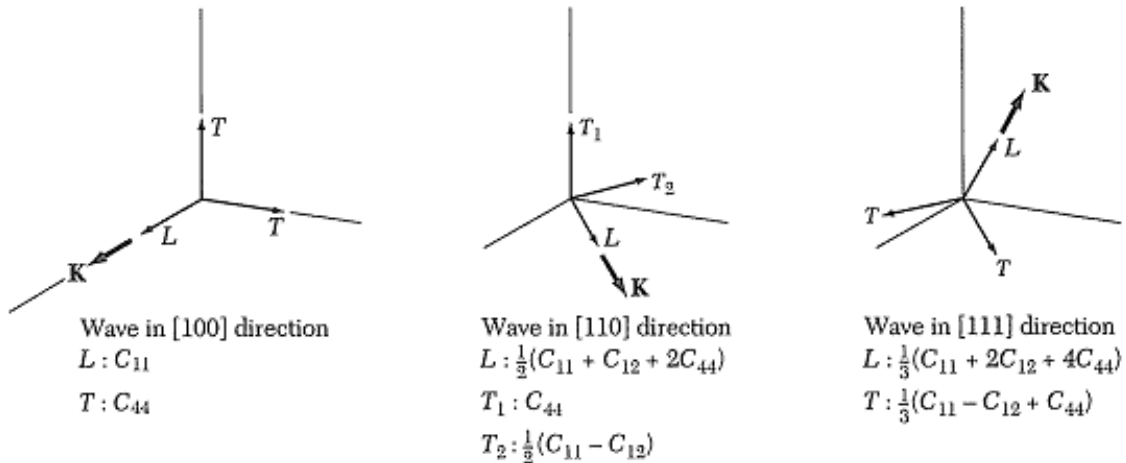
$$\mathbf{k} = \frac{k}{\sqrt{2}}(1,1,0) \qquad \rightarrow \qquad \mathbf{C}_{ij}(\mathbf{k}) = \left(C_{i11j} + C_{i12j} + C_{i21j} + C_{i22j} \right)\frac{k^2}{2}$$

$$\mathbf{C(k)} = \frac{k^2}{2}\begin{pmatrix} C_{1111} + C_{1221} & C_{1122} + C_{1212} & 0 \\ C_{2121} + C_{2211} & C_{2112} + C_{2222} & 0 \\ 0 & 0 & C_{3113} + C_{3223} \end{pmatrix} = \frac{k^2}{2}\begin{pmatrix} C_{11} + C_{44} & C_{12} + C_{44} & 0 \\ C_{12} + C_{44} & C_{11} + C_{44} & 0 \\ 0 & 0 & 2C_{44} \end{pmatrix}$$

$$\omega_L = \sqrt{\frac{1}{2\rho}(C_{11} + C_{12} + 2C_{44})}\; k \qquad \mathbf{u}_0 = (1,1,0) \qquad \text{Lonitudinal}$$

$$\omega_{T1} = \sqrt{\frac{1}{2\rho}(C_{11} - C_{12})}\; k \qquad \mathbf{u}_0 = (1,-1,0) \qquad \text{Transverse}$$

$$\omega_{T2} = \sqrt{\frac{C_{44}}{\rho}}\; k \qquad \mathbf{u}_0 = (0,0,1) \qquad \text{Transverse}$$

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.