Solid state physics - goals

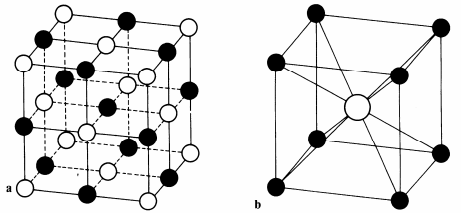
Microscopic understanding of material properties

- *temperature dependence of structure*
- *electric and thermal conductivity*
- *optical properties*
- *magnetization …*

Description of electrons and nuclei in solids, their motion, and their response to external fields

- *10^{23} atoms / cm^3*
- *but: few chemical elements & periodicity*

NaCl

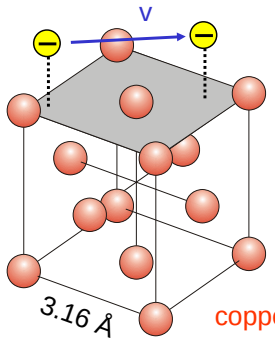


CsCl

Electrons in solids

kinetic energy: E_{kin} = 0.5 eV

velocity v = 1000.000 km / h = 3 Å / fs



Cu(001)

copper (fcc)

Motion on atomic scales:
1 Å = 10^{-10} m
1 fs = 10^{-15} s
h = 4,13 eV fs (Plancksche Konstante)

Pauli principle and Hund´s rules

Periodic Table, with the Outer Electron Configurations of Neutral Atoms in Their Ground States

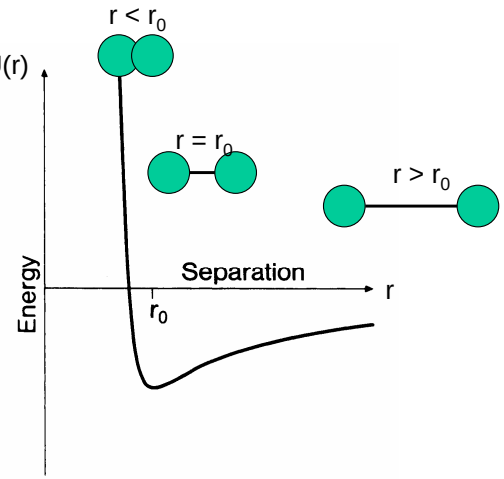
The notation used to describe the electronic configuration of atoms and ions is discussed in all textbooks of introductory atomic physics. The letters *s*, *p*, *d*, . . . signify electrons having orbital angular momentum 0, 1, 2, . . . in units $\hbar$; the number to the left of the letter denotes the principal quantum number of one orbit, and the superscript to the right denotes the number of electrons in the orbit.

H^1 $1s$																	He^2 $1s^2$
Li^3 $2s$	Be^4 $2s^2$											B^5 $2s^22p$	C^6 $2s^22p^2$	N^7 $2s^22p^3$	O^8 $2s^22p^4$	F^9 $2s^22p^5$	Ne^{10} $2s^22p^6$
Na^{11} $3s$	Mg^{12} $3s^2$											Al^{13} $3s^23p$	Si^{14} $3s^23p^2$	P^{15} $3s^23p^3$	S^{16} $3s^23p^4$	Cl^{17} $3s^23p^5$	Ar^{18} $3s^23p^6$
K^{19} $4s$	Ca^{20} $4s^2$	Sc^{21} $3d$ $4s^2$	Ti^{22} $3d^2$ $4s^2$	V^{23} $3d^3$ $4s^2$	Cr^{24} $3d^5$ $4s$	Mn^{25} $3d^5$ $4s^2$	Fe^{26} $3d^6$ $4s^2$	Co^{27} $3d^7$ $4s^2$	Ni^{28} $3d^8$ $4s^2$	Cu^{29} $3d^{10}$ $4s$	Zn^{30} $3d^{10}$ $4s^2$	Ga^{31} $4s^24p$	Ge^{32} $4s^24p^2$	As^{33} $4s^24p^3$	Se^{34} $4s^24p^4$	Br^{35} $4s^24p^5$	Kr^{36} $4s^24p^6$
Rb^{37} $5s$	Sr^{38} $5s^2$	Y^{39} $4d$ $5s^2$	Zr^{40} $4d^2$ $5s^2$	Nb^{41} $4d^4$ $5s$	Mo^{42} $4d^5$ $5s$	Tc^{43} $4d^6$ $5s$	Ru^{44} $4d^7$ $5s$	Rh^{45} $4d^8$ $5s$	Pd^{46} $4d^{10}$ –	Ag^{47} $4d^{10}$ $5s$	Cd^{48} $4d^{10}$ $5s^2$	In^{49} $5s^25p$	Sn^{50} $5s^25p^2$	Sb^{51} $5s^25p^3$	Te^{52} $5s^25p^4$	I^{53} $5s^25p^5$	Xe^{54} $5s^25p^6$
Cs^{55} $6s$	Ba^{56} $6s^2$	La^{57} $5d$ $6s^2$	Hf^{72} $4f^{14}$ $5d^2$ $6s^2$	Ta^{73} $5d^3$ $6s^2$	W^{74} $5d^4$ $6s^2$	Re^{75} $5d^5$ $6s^2$	Os^{76} $5d^6$ $6s^2$	Ir^{77} $5d^9$ –	Pt^{78} $5d^9$ $6s$	Au^{79} $5d^{10}$ $6s$	Hg^{80} $5d^{10}$ $6s^2$	Tl^{81} $6s^26p$	Pb^{82} $6s^26p^2$	Bi^{83} $6s^26p^3$	Po^{84} $6s^26p^4$	At^{85} $6s^26p^5$	Rn^{86} $6s^26p^6$
Fr^{87} $7s$	Ra^{88} $7s^2$	Ac^{89} $6d$ $7s^2$															

Ce^{58} $4f^2$ $6s^2$	Pr^{59} $4f^3$ $6s^2$	Nd^{60} $4f^4$ $6s^2$	Pm^{61} $4f^5$ $6s^2$	Sm^{62} $4f^6$ $6s^2$	Eu^{63} $4f^7$ $6s^2$	Gd^{64} $4f^7$ $5d$ $6s^2$	Tb^{65} $4f^8$ $5d$ $6s^2$	Dy^{66} $4f^{10}$ $6s^2$	Ho^{67} $4f^{11}$ $6s^2$	Er^{68} $4f^{12}$ $6s^2$	Tm^{69} $4f^{13}$ $6s^2$	Yb^{70} $4f^{14}$ $6s^2$	Lu^{71} $4f^{14}$ $5d$ $6s^2$
Th^{90} – $6d^2$ $7s^2$	Pa^{91} $5f^2$ $6d$ $7s^2$	U^{92} $5f^3$ $6d$ $7s^2$	Np^{93} $5f^5$ $7s^2$	Pu^{94} $5f^6$ $7s^2$	Am^{95} $5f^7$ $7s^2$	Cm^{96} $5f^7$ $6d$ $7s^2$	Bk^{97}	Cf^{98}	Es^{99}	Fm^{100}	Md^{101}	No^{102}	Lr^{103}

Concept: ion core (nucleus + inner electrons) & valence electrons

Bonding



bonding (attraction) due to valence electrons
Pauli repulsion between neighbouring atoms

↳ equilibrium distance r_0 (related to lattice parameter)

Crystal binding energy / atom

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 in units kcal per mole, revised to May 4, 1977, after LBL Report 3720 Rev.

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

Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
417.	357.	328.		206.	179.	400.	391.	294.	302.	317.	233.	154.	428.
4.32	3.70	3.40		2.14	1.86	4.14	4.05	3.04	3.14	3.29	2.42	1.60	4.43
99.7	85.3	78.5		49.3	42.8	95.5	93.4	70.2	72.3	75.8	55.8	37.1	102.2
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr
598		536.	456	347.	264.	385							
6.20		5.55	4.73	3.60	2.73	3.99							
142.9		128.	109.	83.0	63.	92.1							

metals: ~1 - 2 eV/atom
covalent: ~3 - 9 eV/atom
ionic: ~6-10 eV/atom

van der Waals: 20-200 meV/atom
hydrogen: ~100 meV/bond

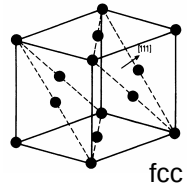
Crystal structure

Table 3 Crystal structures of the elements

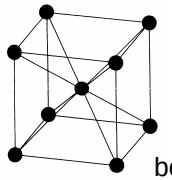
The data given are at room temperature for the most common form, or at the stated temperature in deg K. For further descriptions of the elements see Wyckoff, Vol. 1, Chap. 2. Structures labeled complex are described there.

H[1] 4K																	He[4] 2K
hcp																	hcp
3.75																	3.57
6.12																	5.83
Li 78K	Be											B	C	N 20K	O	F	Ne 4K
bcc	hcp											rhomb.	diamond	cubic	complex		fcc
3.491	2.27												3.567	5.66	(O_2)		4.46
	3.59													(N_2)			
Na 5K	Mg											Al	Si	P	S	Cl	Ar 4K
bcc	hcp	← Crystal structure, →										fcc	diamond	complex	complex	complex	fcc
4.225	3.21	← a lattice parameter, in Å →										4.05	5.430			(Cl_2)	5.31
	5.21	← c lattice parameter, in Å. →															
K 5K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr 4K
bcc	fcc	hcp	hcp	bcc	bcc	cubic	bcc	hcp	fcc	fcc	hcp	complex	diamond	rhomb.	hex.	complex	fcc
5.225	5.58	3.31	2.95	3.03	2.88	complex	2.87	2.51	3.52	3.61	2.66		5.658		chains	(Br_2)	5.64
		5.27	4.68					4.07			4.95						
Rb 5K	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn (α)	Sb	Te	I	Xe 4K
bcc	fcc	hcp	hcp	bcc	bcc	hcp	hcp	fcc	fcc	fcc	hcp	tetr.	diamond	rhomb.	hex.	complex	fcc
5.585	6.08	3.65	3.23	3.30	3.15	2.74	2.71	3.80	3.89	4.09	2.98	3.25	6.49		chains	(I_2)	6.13
		5.73	5.15			4.40	4.28				5.62	4.95					
Cs 5K	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
bcc	bcc	hex.	hcp	bcc	bcc	hcp	hcp	fcc	fcc	fcc	rhomb.	hcp	fcc	rhomb.	sc		
6.045	5.02	3.77	3.19	3.30	3.16	2.76	2.74	3.84	3.92	4.08		3.46	4.95		3.34	—	—
		ABAC	5.05			4.46	4.32					5.52					
Fr	Ra	Ac															
—	—	fcc															
		5.31															

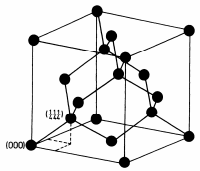
Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
fcc	hex.	hex.	—	complex	bcc	hcp	hcp	hcp	hcp	hcp	hcp	fcc	hcp
5.16	3.67	3.66			4.58	3.63	3.60	3.59	3.58	3.56	3.54	5.48	3.50
	ABAC					5.78	5.70	5.65	5.62	5.59	5.56		5.55
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr
fcc	tetr.	complex	complex	complex	hex.	—	—	—	—	—	—	—	—
5.08	3.92				3.64								
	3.24				ABAC								



fcc

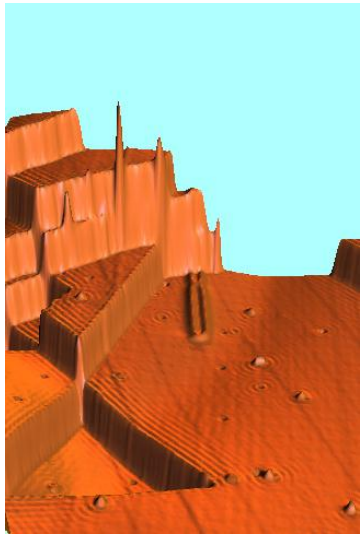


bcc



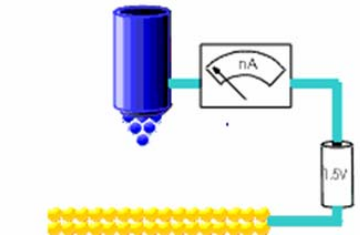
diamond

Wave-particle dualism

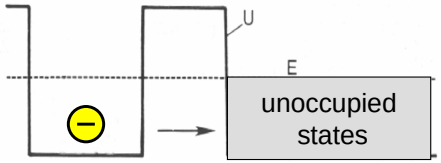


[Crommie, Lutz, Eigler]

http://www.almaden.ibm.com/vis/stm/gallery.html



tunnel current



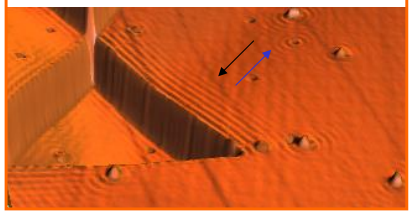
Electron waves

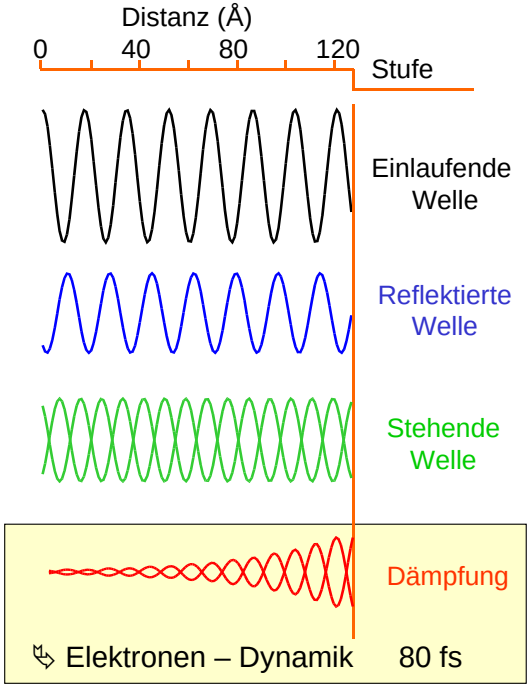
Louis de Broglie (1924):
Wave character of matter

$$p = \frac{h}{\lambda}$$

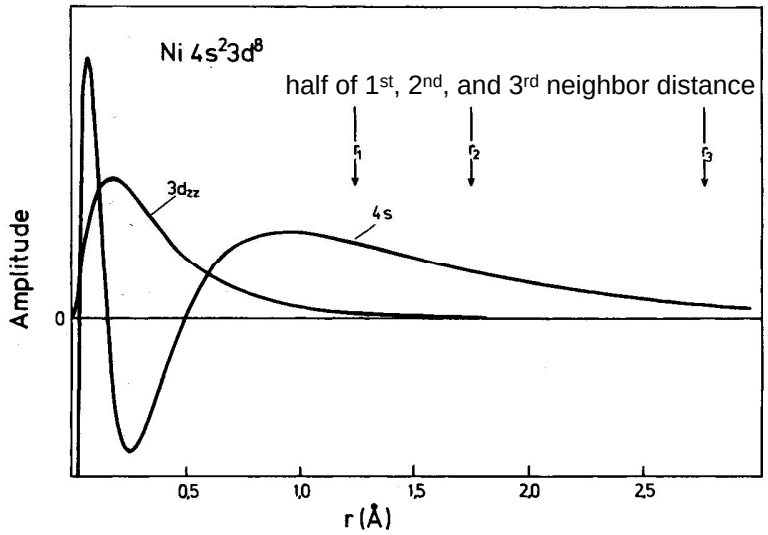
elektron: $E_{kin} = 0.5$ eV

$\lambda = 17.3$ Å





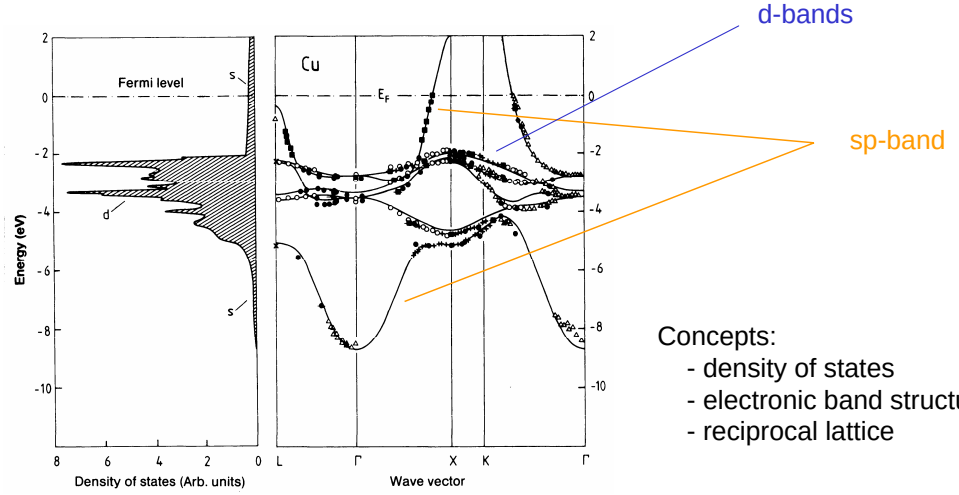
Metallic bonding



Radial part of the wave function of Ni 3s and $3d_{z2}$

Valence bands

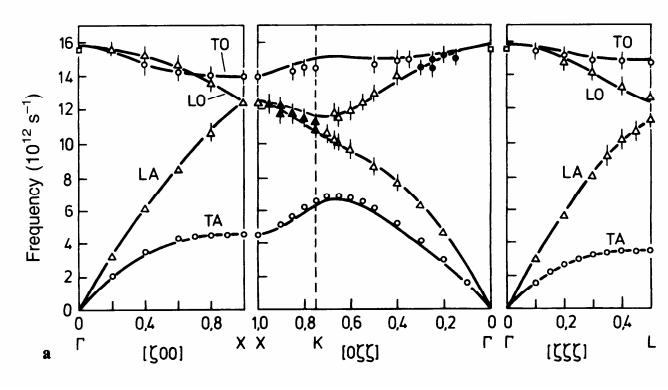
Density of states Dispersion relation E(k)



Concepts:
- density of states
- electronic band structure
- reciprocal lattice

Vibration of atoms in solids - phonons

Atoms vibrate around their equilibrium position r_0 in potential U(r)
- nearly harmonic oscillations
- influence on neighboring atoms leads to collective vibrations
- quantized normal modes: *phonons*



silicon

- longitudinal (L) and transversal (T) modes
- acoustic (A) and optical (O) phonons

Inhalt