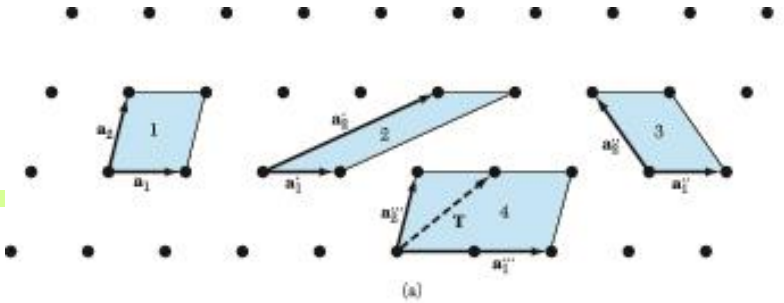
Introduction to Solid State Physics
(C. Kittel)

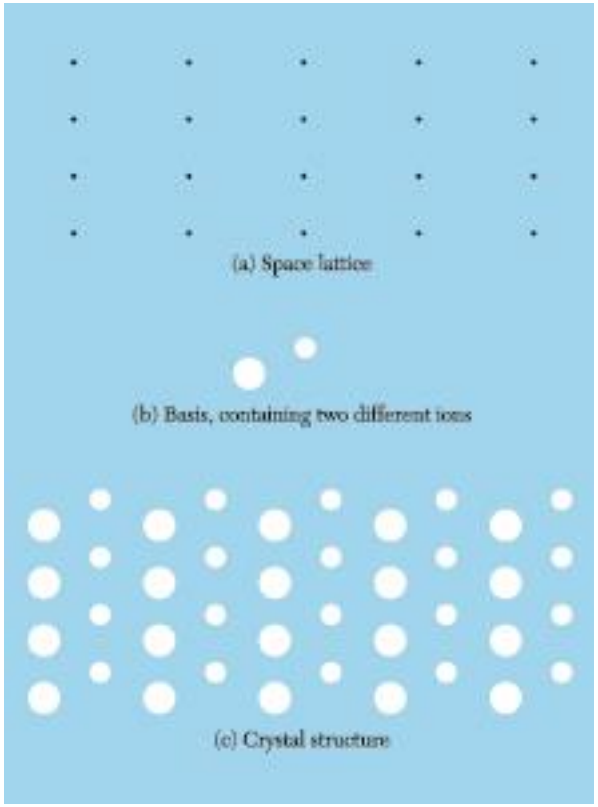
Chapter 1

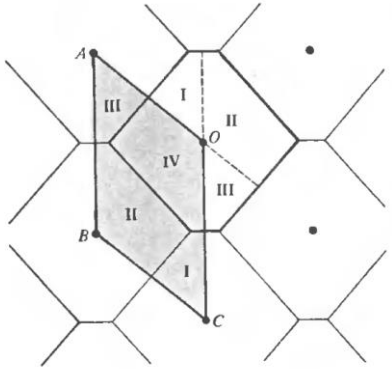
Contents

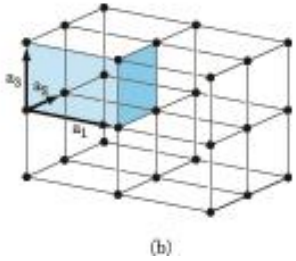
Periodic Array of Atoms

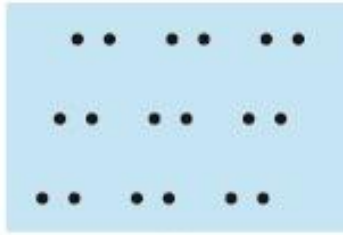


Crystal = Lattice + Basis



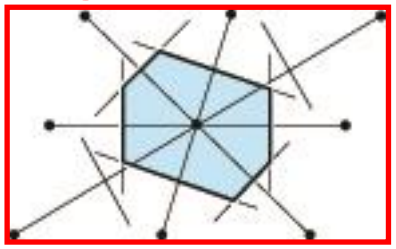






not all lattice points

Wigner-Seitz cell



"primitive"

$\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$: lattice basis vectors

Lattice cell volume

$$V_c = |\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3| \ ,$$

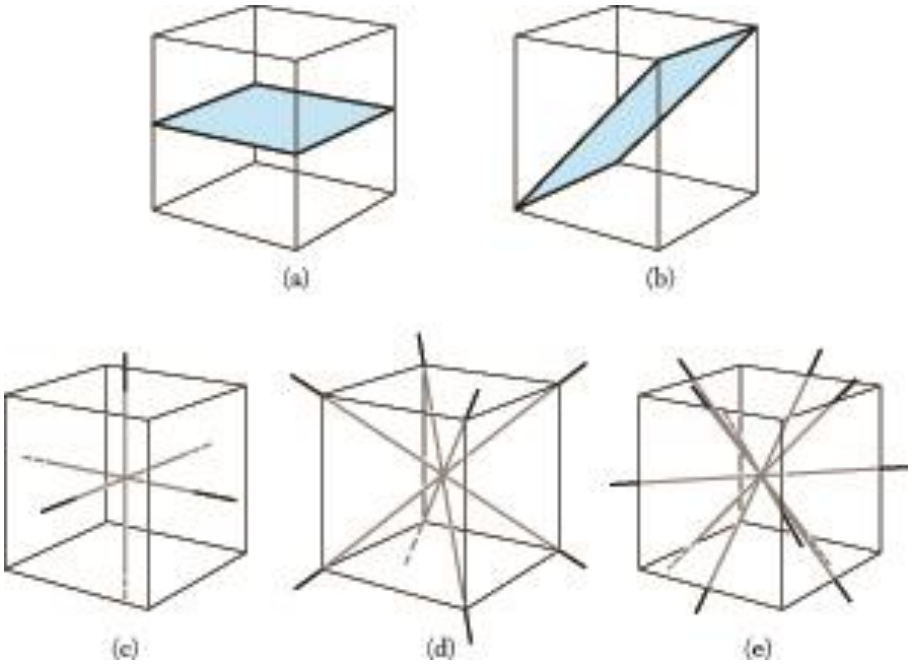
Lattice translation vectors $\mathbf{r}' = \mathbf{r} + u_1\mathbf{a}_1 + u_2\mathbf{a}_2 + u_3\mathbf{a}_3$. u_1, u_2, u_3 are arbitrary integers.

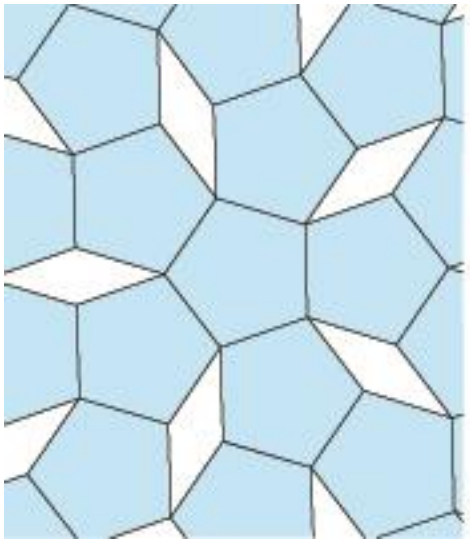
Position of basis $\mathbf{r}_j = x_j\mathbf{a}_1 + y_j\mathbf{a}_2 + z_j\mathbf{a}_3$. $0 \le x_j, y_j, z_j \le 1$.

Fundamental Types of Lattices

Bravais lattice

Symmetries: translation, mirror (reflection), rotation, inversion



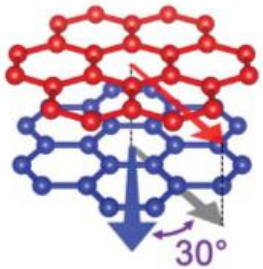


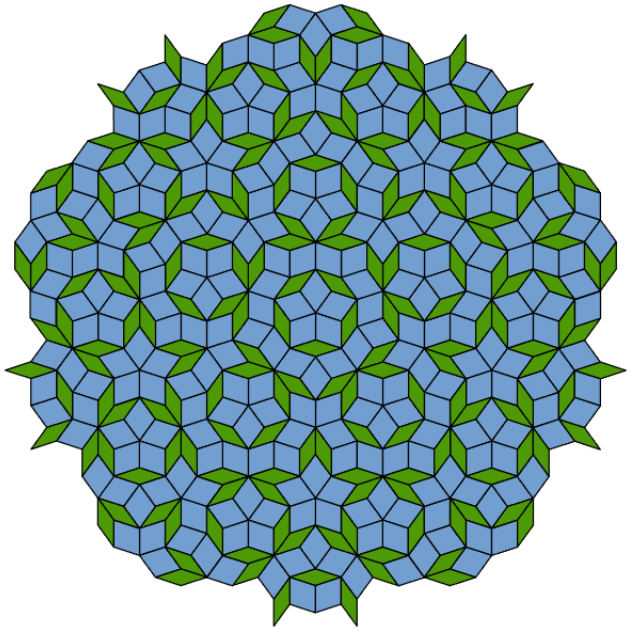
Rotational symmetries in crystals
: 1, 2, 3, 4, 6-fold symmetric

5-fold, 10-fold quasi-symmetric
➔ quasi-crystals (some metal alloys)

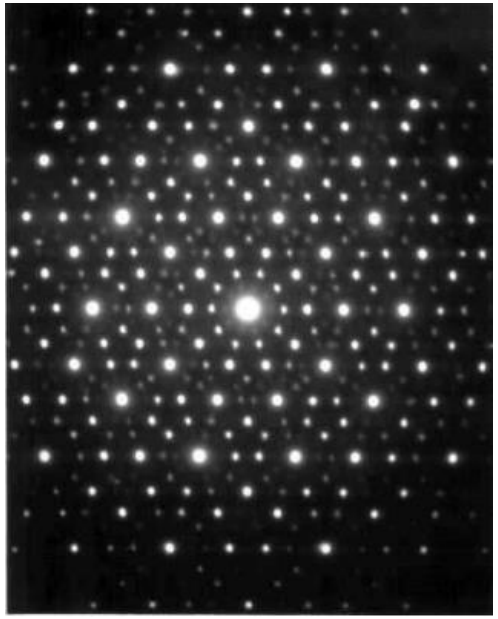
Fundamental Types of Lattices

5-fold, 10-fold quasi-symmetric
→ quasi-crystals (some metal alloys)

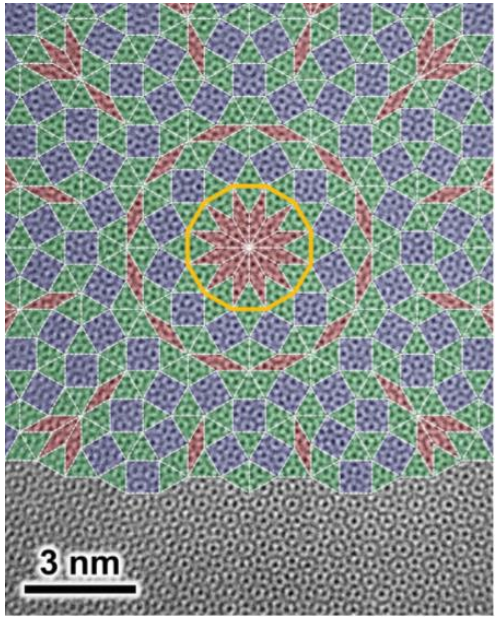




Penrose 2D tiling



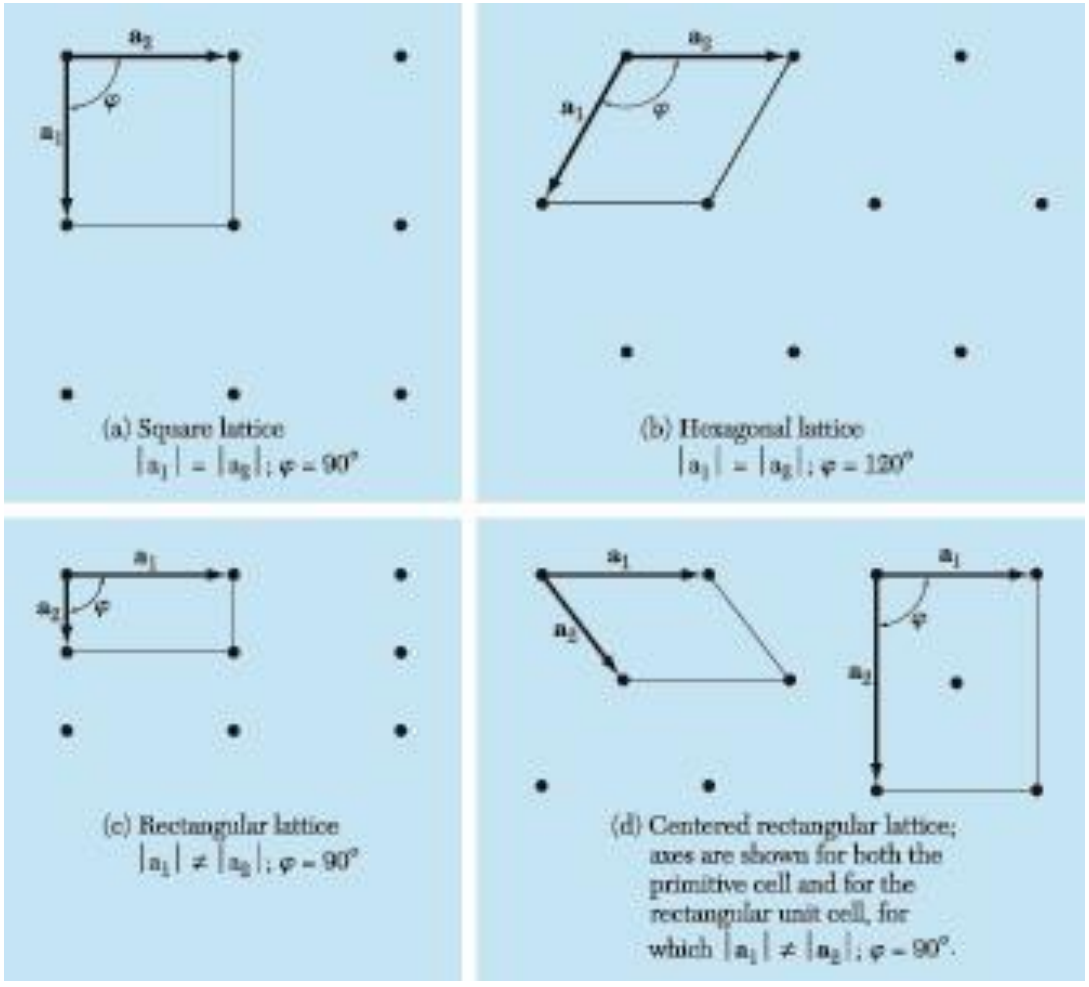
electron diffraction (TEM) from $Al_{86}Mn_{14}$ alloy (1984)
***k*-space**



TEM from graphene quasicrystal (2018)
***R*-space**

Fundamental Types of Lattices

Fundamental types of lattices : 5 in 2D (14 in 3D)

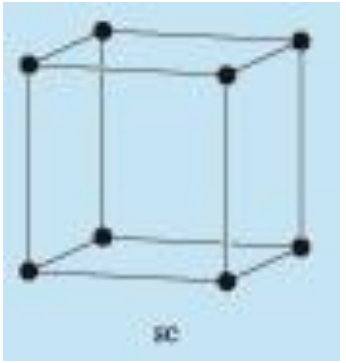


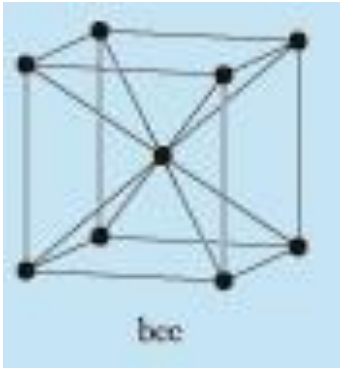
Fundamental Types of Lattices

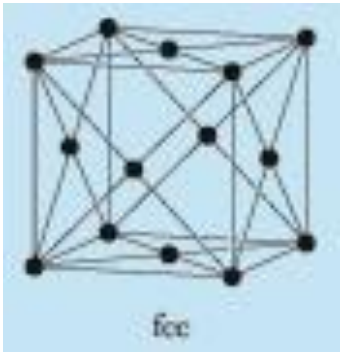
Fundamental types of lattices : 14 in 3D

Table 1 The 14 lattice types in three dimensions

System	Number of lattices	Restrictions on conventional cell axes and angles
Triclinic	1	$a_1 \neq a_2 \neq a_3$ $\alpha \neq \beta \neq \gamma$
Monoclinic	2	$a_1 \neq a_2 \neq a_3$ $\alpha = \gamma = 90° \neq \beta$
Orthorhombic	4	$a_1 \neq a_2 \neq a_3$ $\alpha = \beta = \gamma = 90°$
Tetragonal	2	$a_1 = a_2 \neq a_3$ $\alpha = \beta = \gamma = 90°$
Cubic	3	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90°$
Trigonal	1	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma < 120°, \neq 90°$
Hexagonal	1	$a_1 = a_2 \neq a_3$ $\alpha = \beta = 90°$ $\gamma = 120°$

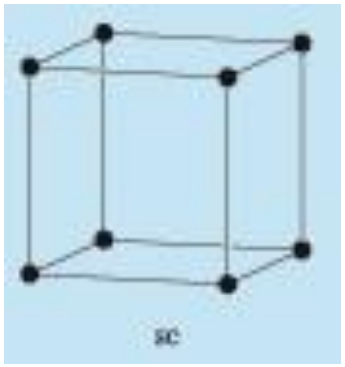


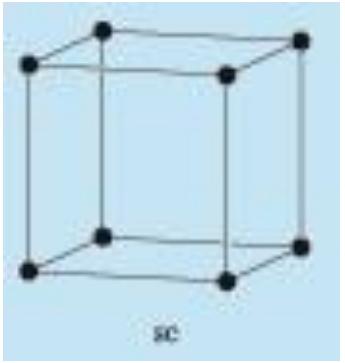




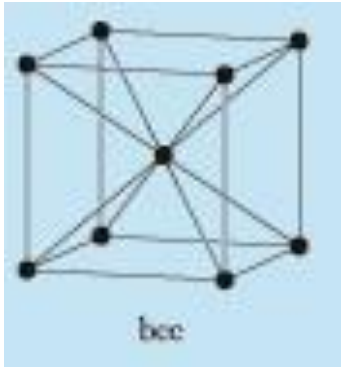
3 Cubic types of Lattices

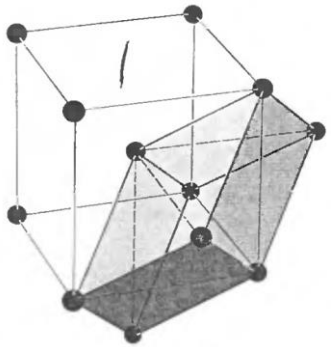
Conventional unit cell | **Primitive unit cell** | **Wigner-Seitz cell**



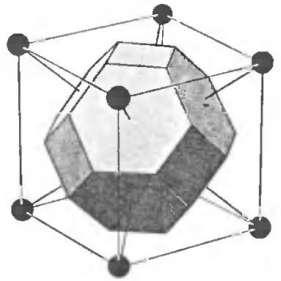


cubic with same size with a lattice point at the center

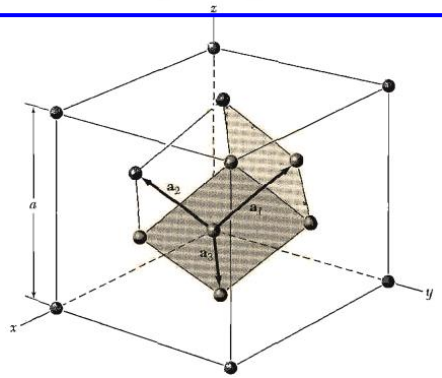




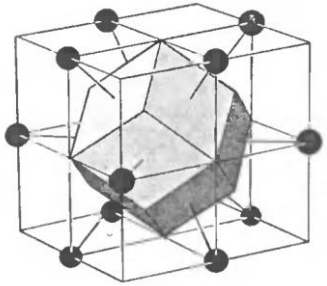
$$\mathbf{a}_1 = \tfrac{1}{2}a(-\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$$
$$\mathbf{a}_2 = \tfrac{1}{2}a(\hat{\mathbf{x}} - \hat{\mathbf{y}} + \hat{\mathbf{z}})\ ;$$
$$\mathbf{a}_3 = \tfrac{1}{2}a(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}})$$



“truncated octahedron”



$$\mathbf{a}_1 = \frac{1}{2}a(\hat{\mathbf{y}} + \hat{\mathbf{z}})$$
$$\mathbf{a}_2 = \frac{1}{2}a(\hat{\mathbf{x}} + \hat{\mathbf{z}})$$
$$\mathbf{a}_3 = \frac{1}{2}a(\hat{\mathbf{x}} + \hat{\mathbf{y}})$$

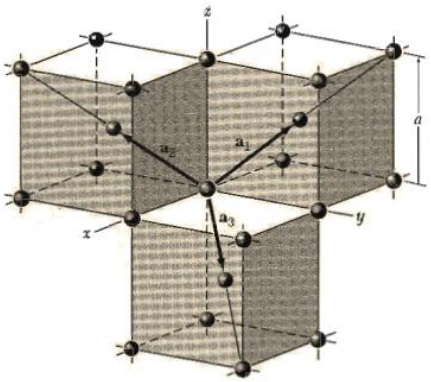


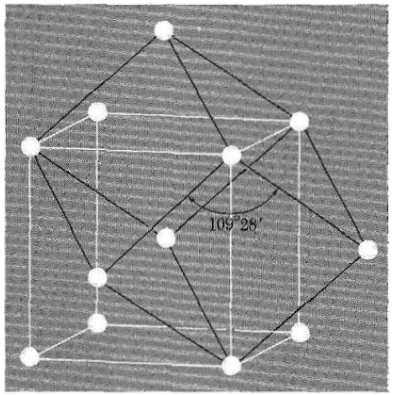
“rhombic dodecahedron”

3 Cubic types of Lattices

The primitive translation vectors of the bcc lattice (Fig. 12) are

$$\mathbf{a}_1 = \tfrac{1}{2}a(-\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}) \; ; \quad \mathbf{a}_2 = \tfrac{1}{2}a(\hat{\mathbf{x}} - \hat{\mathbf{y}} + \hat{\mathbf{z}}) \; ; \quad \mathbf{a}_3 = \tfrac{1}{2}a(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}) \; ,$$

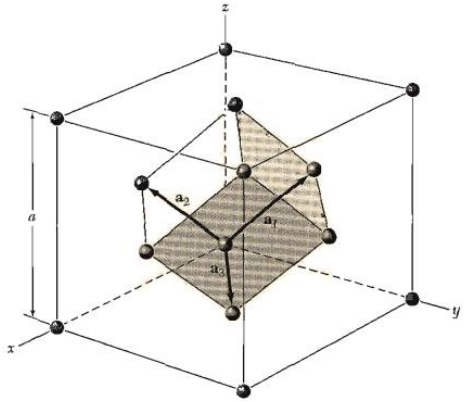




$$V = |\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3| = \tfrac{1}{2}a^3$$

The primitive translation vectors of the fcc lattice of Fig. 14 are

$$\mathbf{a}_1 = \frac{1}{2}a(\hat{\mathbf{y}} + \hat{\mathbf{z}}) \; ; \quad \mathbf{a}_2 = \frac{1}{2}a(\hat{\mathbf{x}} + \hat{\mathbf{z}}) \; ; \quad \mathbf{a}_3 = \frac{1}{2}a(\hat{\mathbf{x}} + \hat{\mathbf{y}}) \; .$$



$$V = |\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3| = \frac{1}{4}a^3$$

3 Cubic types of Lattices

Table 2 Characteristics of cubic lattices[a]

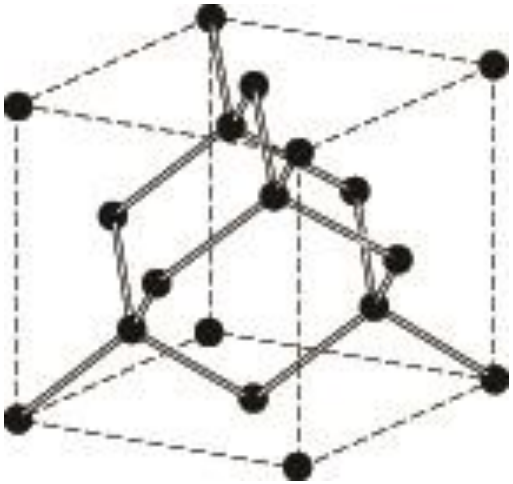
	Simple	Body-centered	Face-centered
Volume, conventional cell	a^3	a^3	a^3
Lattice points per cell	1	2	4
Volume, primitive cell	a^3	$\frac{1}{2}a^3$	$\frac{1}{4}a^3$
Lattice points per unit volume	$1/a^3$	$2/a^3$	$4/a^3$
Number of nearest neighbors	6	8	12
Nearest-neighbor distance	a	$3^{1/2}\,a/2 = 0.866a$	$a/2^{1/2} = 0.707a$
Number of second neighbors	12	6	6
Second neighbor distance	$2^{1/2}a$	a	a
Packing fraction[a]	$\frac{1}{6}\pi$ $=0.524$	$\frac{1}{8}\pi\sqrt{3}$ $=0.680$	$\frac{1}{6}\pi\sqrt{2}$ $=0.740$

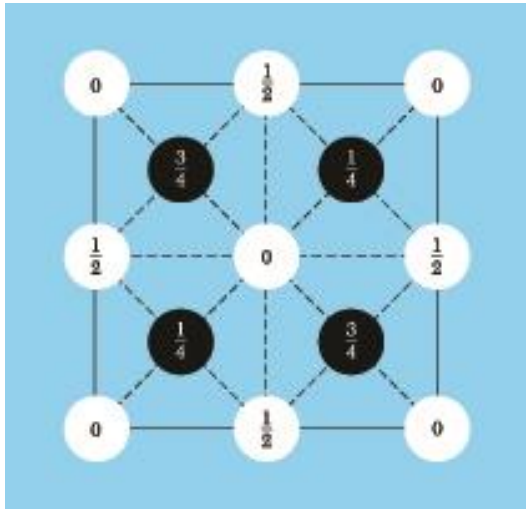
[a] The packing fraction is the maximum proportion of the available volume that can be filled with hard spheres.

Homework: Check all by yourself!

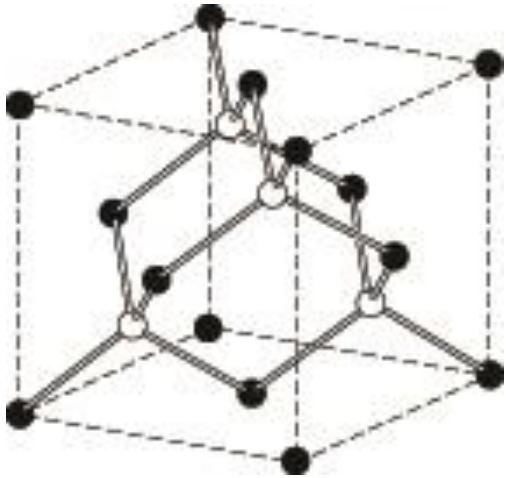
Simple Crystal Structures

diamond structure (C, Si, Ge)





ZnS structure (SiC, ZnS,GaAs, GaP…)
: III-V compound semiconductors

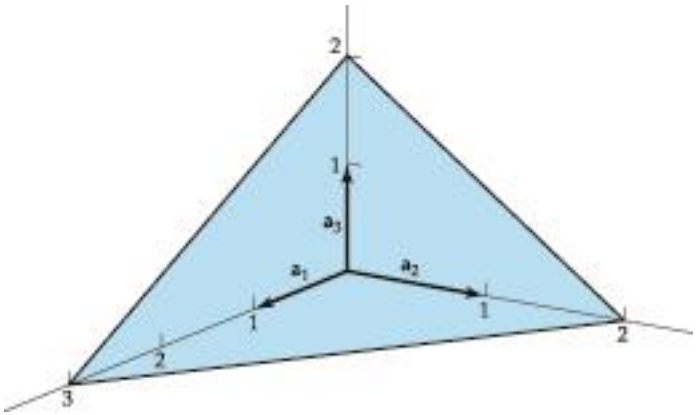


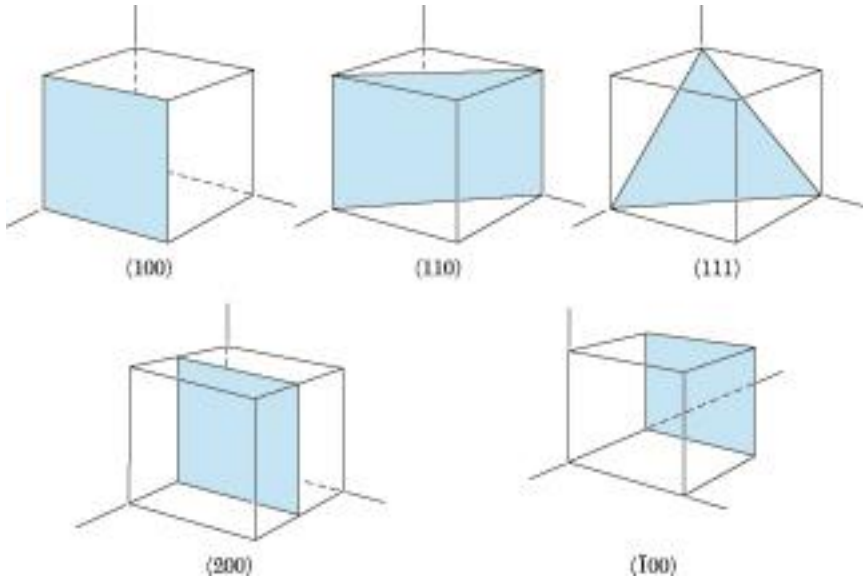
Quiz: For each structure,
(i) Lattice structure?
(ii) # of basis atoms?

Index Systems for Crystal Planes : Miller Index

- Find the intercepts on the axes in terms of the lattice constants a_1, a_2, a_3. The axes may be those of a primitive or nonprimitive cell.

- Take the reciprocals of these numbers and then reduce to three integers having the same ratio, usually the smallest three integers. The result, enclosed in parentheses (hkl), is called the index of the plane.

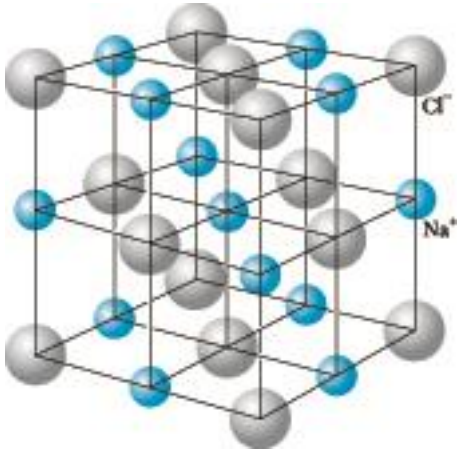




Simple Crystal Structures

Homework: For each structure,
(i) Lattice structure?
(ii) # of basis atoms?

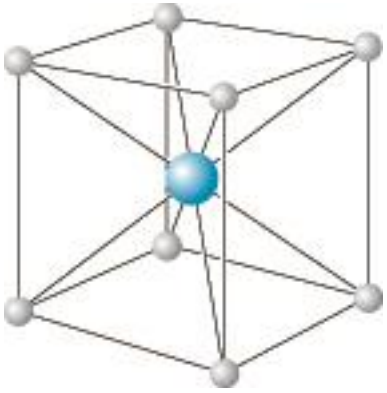
NaCl structure



Cl:	000 ;	$\frac{1}{2}\frac{1}{2}0$;	$\frac{1}{2}0\frac{1}{2}$;	$0\frac{1}{2}\frac{1}{2}$.
Na:	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$;	$00\frac{1}{2}$;	$0\frac{1}{2}0$;	$\frac{1}{2}00$.

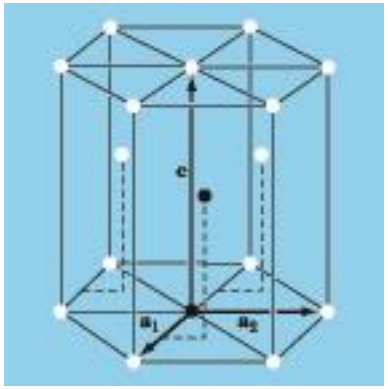
Crystal	a	Crystal	a
LiH	4.08 Å	AgBr	5.77 Å
MgO	4.20	PbS	5.92
MnO	4.43	KCl	6.29
NaCl	5.63	KBr	6.59

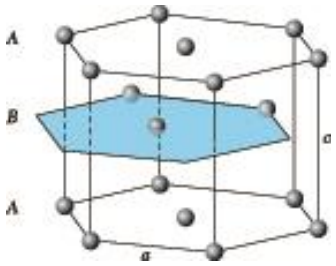
CsCl structure



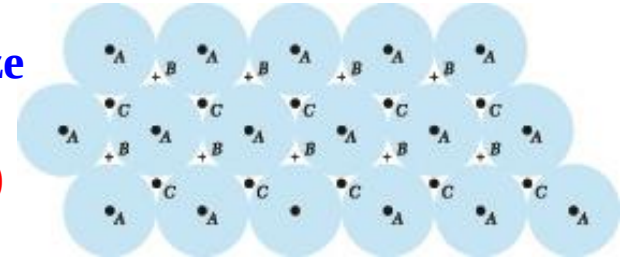
hcp structure

simple hexagonal lattice





Atom stacking to maximize the packing fraction
➔ **close packing (fcc, hcp)**



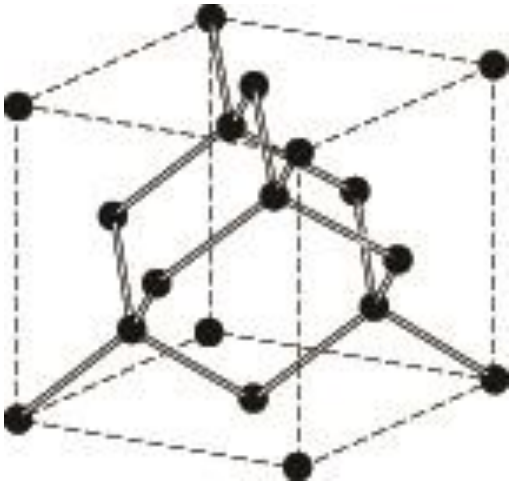
Binding energy depends on "coordination" number

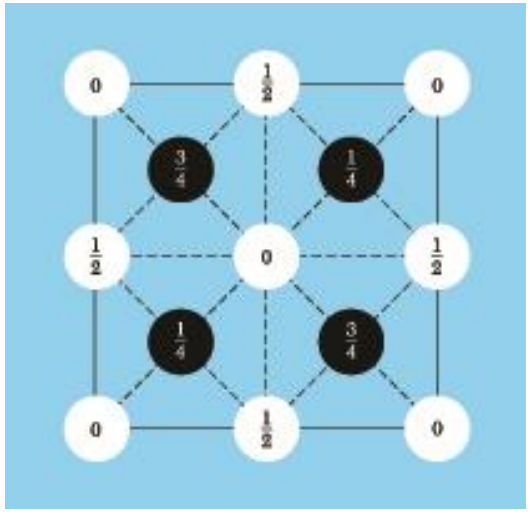
Random Stacking and Polytypism

Simple Crystal Structures

Homework: For each structure,
(i) Lattice structure?
(ii) # of basis atoms?

diamond structure (C, Si, Ge)





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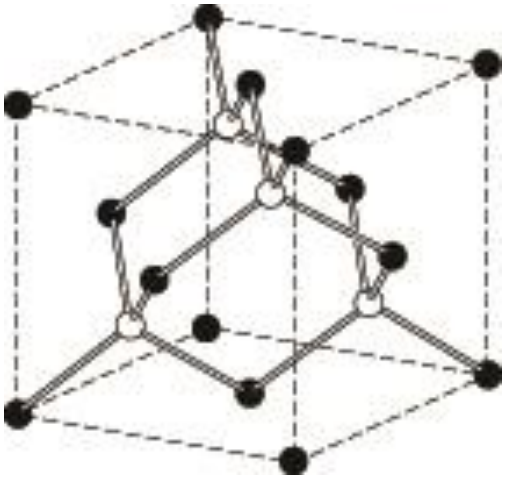


Crystal Structures of Elements

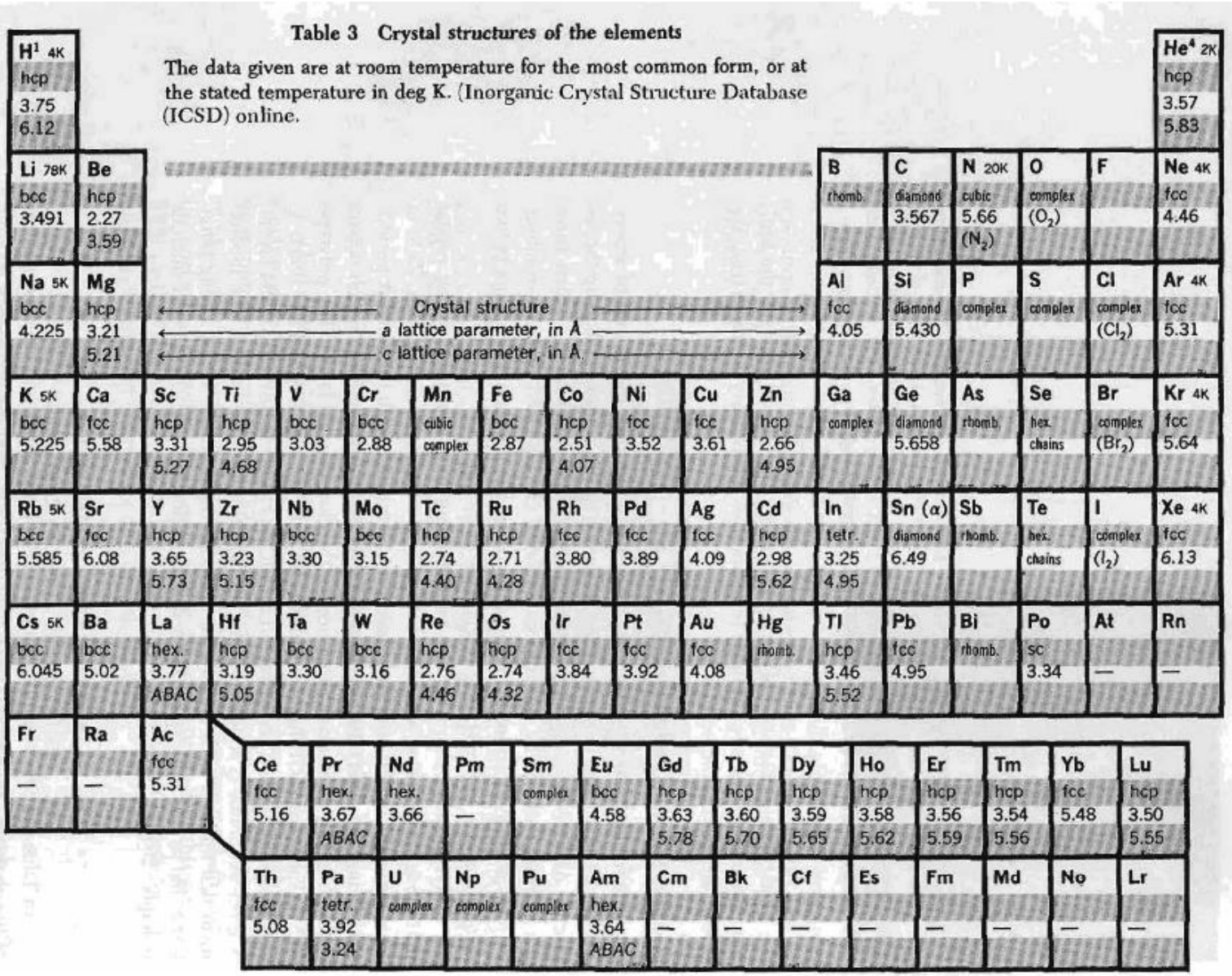


Table 3 Crystal structures of the elements

The data given are at room temperature for the most common form, or at the stated temperature in deg K. (Inorganic Crystal Structure Database (ICSD) online.

Crystal structure
a lattice parameter, in Å
c lattice parameter, in Å

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

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

보충

Looking at atoms in real space - *Microscope*

in real space → microscopes

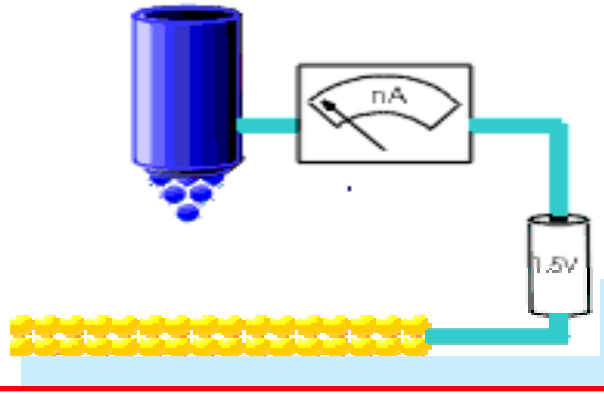
- Transmission Electron Microscope (TEM)
- Scanning Tunelling Microscope (STM)
- Atomic Force microscope (AFM)

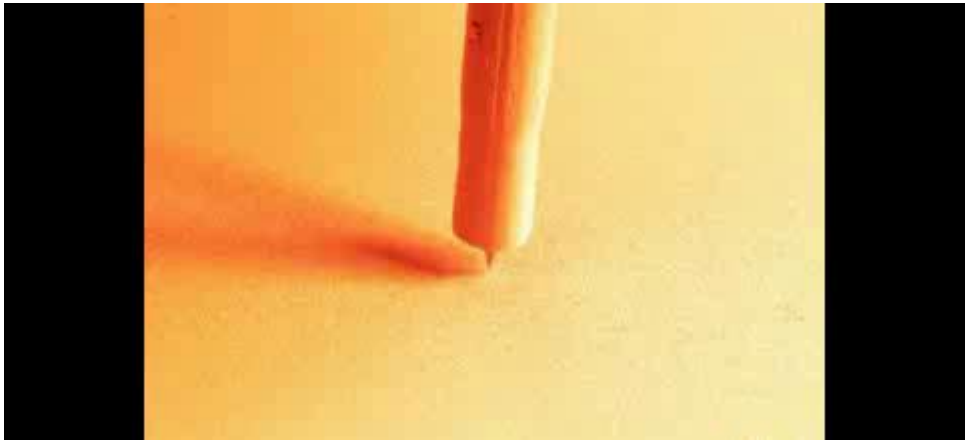
in momentum space → diffractions

- X-ray diffraction (XRD)
- neutron scattering
- Atom scattering
- Low-energy electron diffraction (LEED)

Ex. STM

Simple schematic

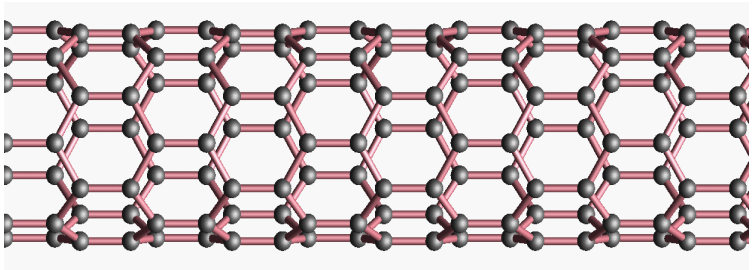


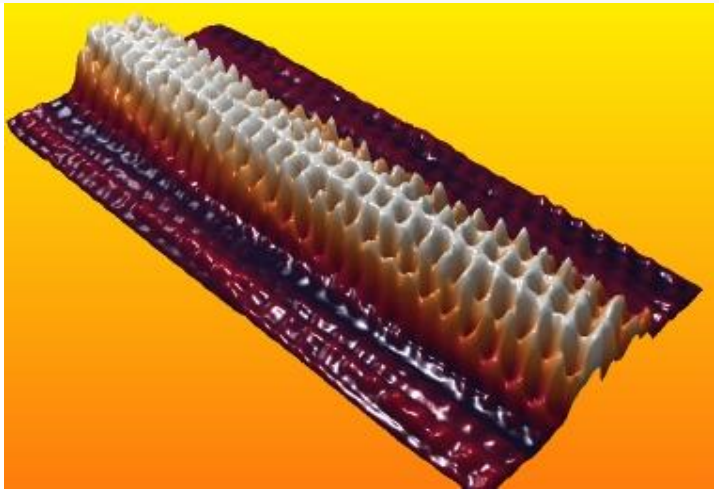


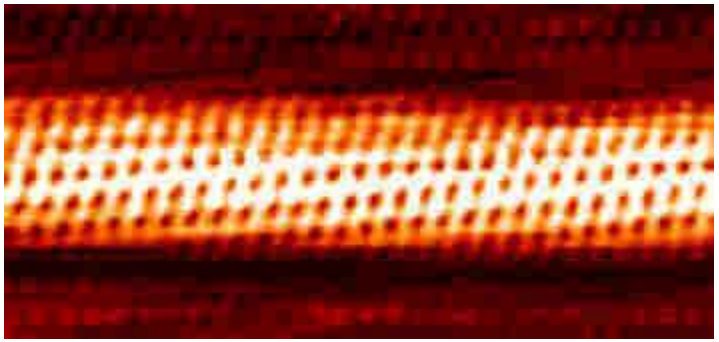
보충

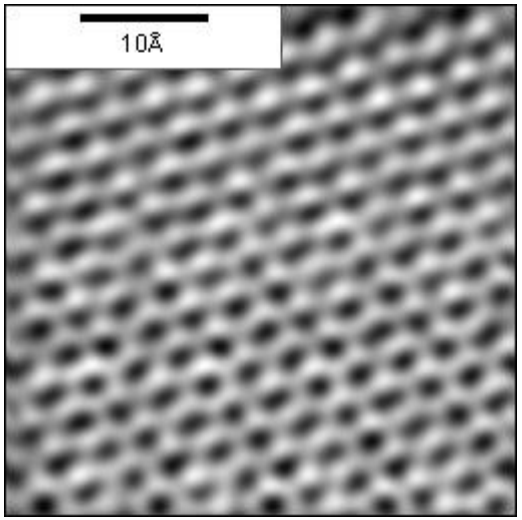
Looking at atoms - *STM images*

CNT

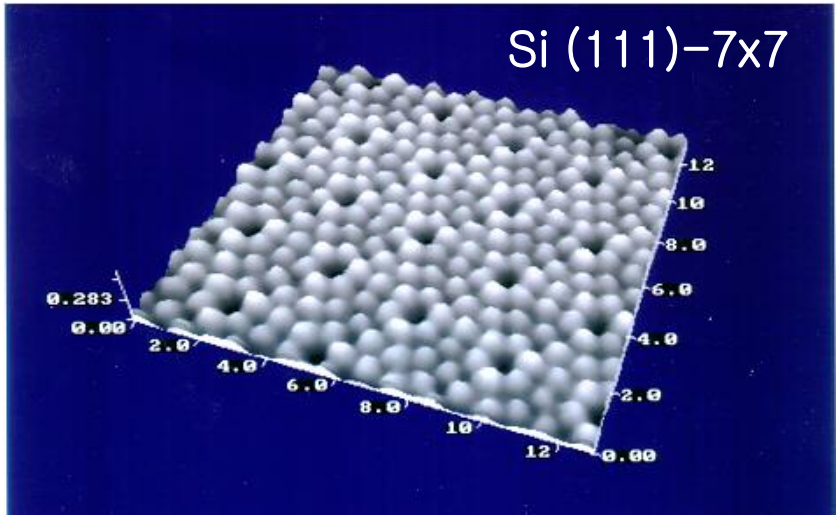








Cu (111)



SUMMARY

SUMMARY

- A lattice is an array of points related by the lattice translation operator $\mathbf{T} = u_1\mathbf{a}_1 + u_2\mathbf{a}_2 + u_3\mathbf{a}_3$, where u_1, u_2, u_3 are integers and $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ are the crystal axes.
- To form a crystal we attach to every lattice point an identical basis composed of s atoms at the positions $\mathbf{r}_j = x_j\mathbf{a}_1 + y_j\mathbf{a}_2 + z_j\mathbf{a}_3$, with $j = 1, 2, \ldots, s$. Here x, y, z may be selected to have values between 0 and 1.
- The axes $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ are primitive for the minimum cell volume $|\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3|$ for which the crystal can be constructed from a lattice translation operator $\mathbf{T}$ and a basis at every lattice point.

Homework

Problems #1~3