

SIXTH EDITION

KITTEL

Introduction to Solid State Physics

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About the Author

Charles Kittel taught solid state physics at Berkeley from 1951 to 1978; earlier he was a member of the solid state group at the Bell Laboratories. His undergraduate work was at M.I.T. and at Cambridge University, followed by graduate work at the University of Wisconsin. He is a member of the National Academy of Science and of the American Academy of Arts and Sciences.

His research in solids began with studies of ferromagnetic, antiferromagnetic, and paramagnetic resonance, along with work on magnetic domains, spin waves, and domain boundaries in ferromagnets and ferroelectrics. His work on the single domain structure of fine particles was paralleled by that of L. Néel and has had broad application in magnetic recording. Along with collaborators at Berkeley he worked on cyclotron resonance in semiconductors, which led to the first understanding of the band structure of silicon, germanium, and indium antimonide, together with the theory of their impurity states. He also worked on the interpretation of magnetoplasma resonance in semiconductors and of Alfvén resonance in electron-hole drops in germanium.

The first edition of *ISSP* was the first textbook to integrate the elementary aspects of solid state physics for study by seniors and beginning graduate students. Now in its sixth edition, *ISSP* plays the same part for the current generation of students.

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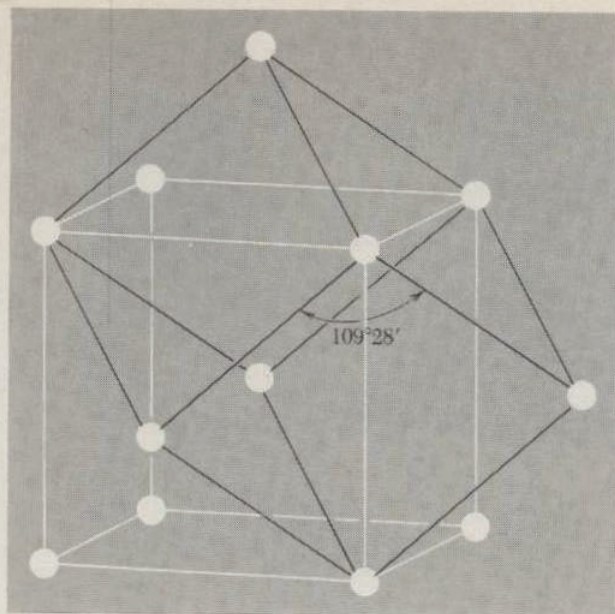


Figure 11 Body-centered cubic lattice, showing a primitive cell. The primitive cell shown is a rhombohedron of edge $\frac{1}{2}\sqrt{3}a$, and the angle between adjacent edges is $109^{\circ}28'$.

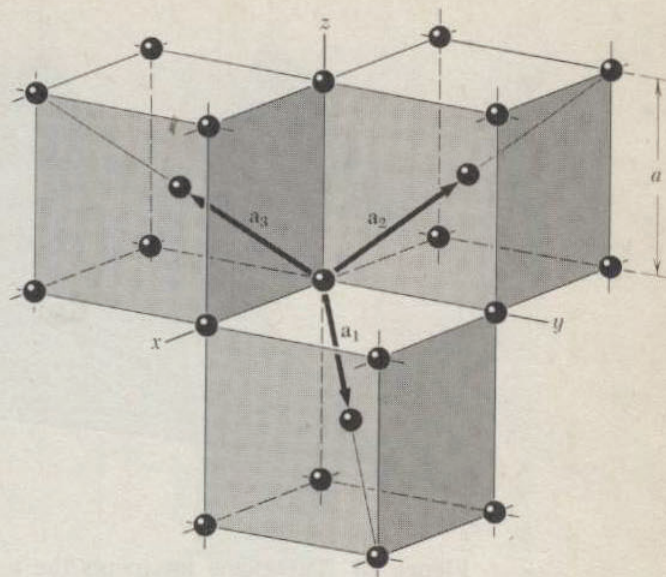


Figure 12 Primitive translation vectors of the body-centered cubic lattice; these vectors connect the lattice point at the origin to lattice points at the body centers. The primitive cell is obtained on completing the rhombohedron. In terms of the cube edge a the primitive translation vectors are

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a(\hat{x} + \hat{y} - \hat{z}) ; & \mathbf{a}_2 &= \frac{1}{2}a(-\hat{x} + \hat{y} + \hat{z}) ; \\ \mathbf{a}_3 &= \frac{1}{2}a(\hat{x} - \hat{y} + \hat{z}) . \end{aligned}$$

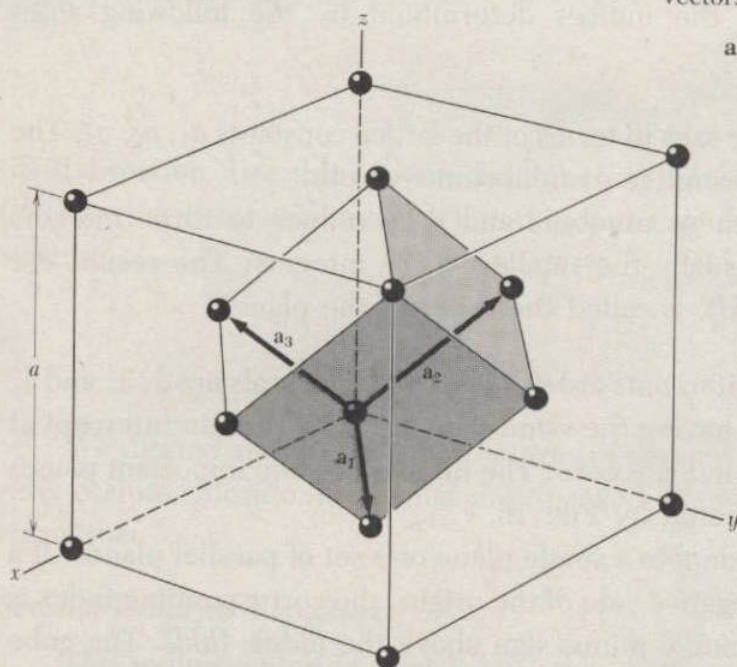


Figure 13 The rhombohedral primitive cell of the face-centered cubic crystal. The primitive translation vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ connect the lattice point at the origin with lattice points at the face centers. As drawn, the primitive vectors are:

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

The angles between the axes are 60° . Here $\hat{x}$, $\hat{y}$, $\hat{z}$ are the Cartesian unit vectors.

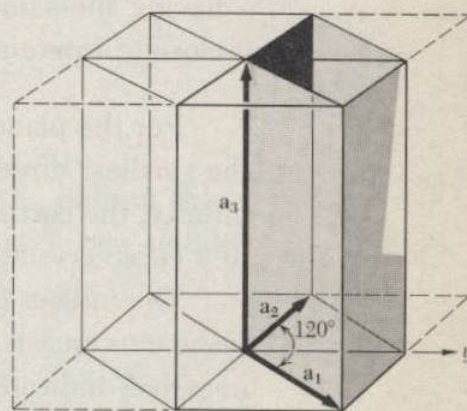


Figure 14 Relation of the primitive cell in the hexagonal system (heavy lines) to a prism of hexagonal symmetry. Here $a_1 = a_2 \neq a_3$.

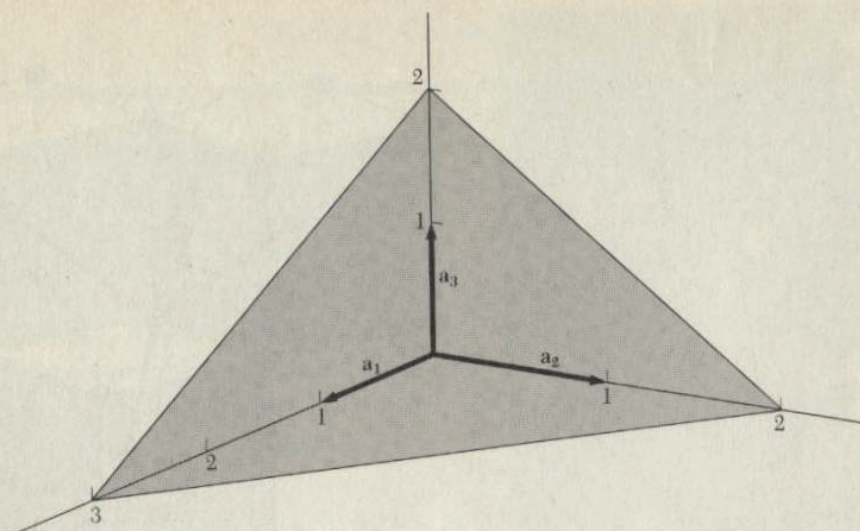


Figure 15 This plane intercepts the a_1 , a_2 , a_3 axes at $3a_1$, $2a_2$, a_3 . The reciprocals of these numbers are $\frac{1}{3}$, $\frac{1}{2}$, $\frac{1}{1}$. The smallest three integers having the same ratio are 2, 3, 3, and thus the indices of the plane are (233).

However, it turns out to be more useful for structure analysis to specify the orientation of a plane by the indices determined by the following rules (Fig. 15).

- 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.

For the plane whose intercepts are 4, 1, 2, the reciprocals are $\frac{1}{4}$, 1, and $\frac{1}{2}$; the smallest three integers having the same ratio are (142). For an intercept at infinity, the corresponding index is zero. The indices of some important planes in a cubic crystal are illustrated by Fig. 16.

The indices (hkl) may denote a single plane or a set of parallel planes. If a plane cuts an axis on the negative side of the origin, the corresponding index is negative, indicated by placing a minus sign above the index: ($h\bar{k}l$). The cube faces of a cubic crystal are (100), (010), (001), ($\bar{1}00$), ($0\bar{1}0$), and ($00\bar{1}$). Planes equivalent by symmetry may be denoted by curly brackets (braces) around indices; the set of cube faces is {100}. When we speak of the (200) plane we mean a plane parallel to (100) but cutting the a_1 axis at $\frac{1}{2}a$.

The indices $[uvw]$ of a direction in a crystal are the set of the smallest integers that have the ratio of the components of a vector in the desired direction, referred to the axes. The a_1 axis is the [100] direction; the $-a_2$ axis is the

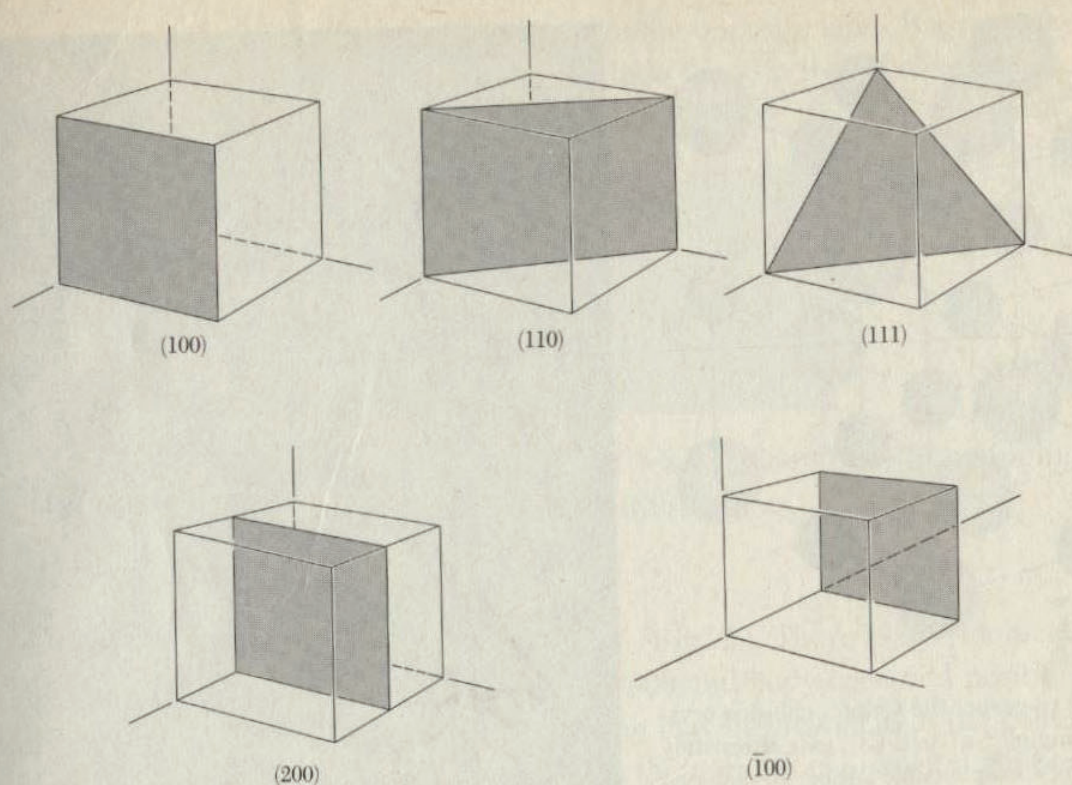


Figure 16 Indices of important planes in a cubic crystal. The plane (200) is parallel to (100) and to $(\bar{1}00)$.

$[0\bar{1}0]$ direction. In cubic crystals the direction $[hkl]$ is perpendicular to a plane (hkl) having the same indices, but this is not generally true in other crystal systems.

SIMPLE CRYSTAL STRUCTURES

We discuss simple crystal structures of general interest: the sodium chloride, cesium chloride, hexagonal close-packed, diamond, and cubic zinc sulfide structures.

Sodium Chloride Structure

The sodium chloride, NaCl, structure is shown in Figs. 17 and 18. The lattice is face-centered cubic; the basis consists of one Na atom and one Cl atom separated by one-half the body diagonal of a unit cube. There are four units of NaCl in each unit cube, with atoms in the positions

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

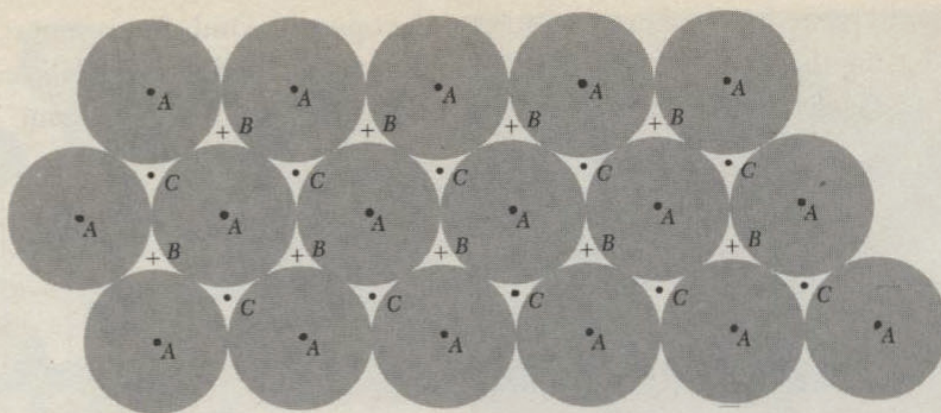


Figure 21 A close-packed layer of spheres is shown, with centers at points marked A. A second and identical layer of spheres can be placed on top of this, above and parallel to the plane of the drawing, with centers over the points marked B. There are two choices for a third layer. It can go in over A or over C. If it goes in over A the sequence is ABABAB. . . and the structure is hexagonal close-packed. If the third layer goes in over C the sequence is ABCABCABC. . . and the structure is face-centered cubic.

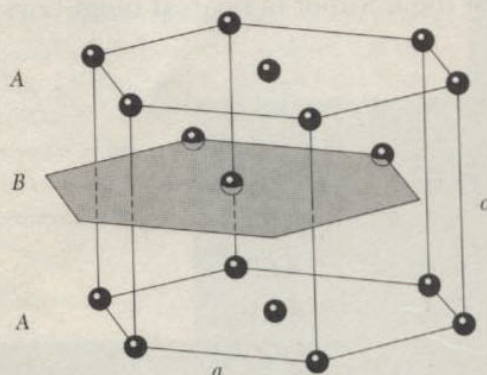


Figure 22 The hexagonal close-packed structure. The atom positions in this structure do not constitute a space lattice. The space lattice is simple hexagonal with a basis of two identical atoms associated with each lattice point. The lattice parameters a and c are indicated, where a is in the basal plane and c is the magnitude of the axis $\mathbf{a}_3$ of Fig. 14.

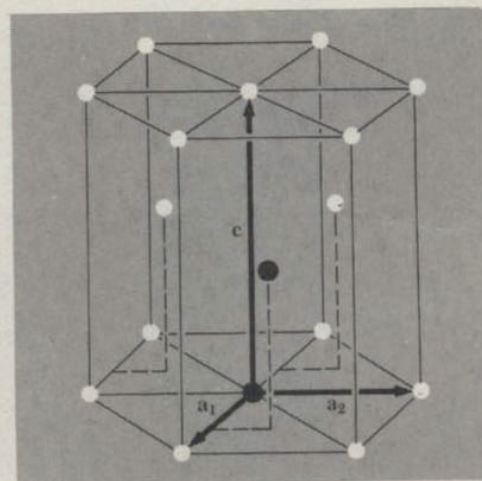


Figure 23 The primitive cell has $a_1 = a_2$, with an included angle of 120° . The c axis (or $\mathbf{a}_3$) is normal to the plane of $\mathbf{a}_1$ and $\mathbf{a}_2$. The ideal hcp structure has $c = 1.633 a$. The two atoms of one basis are shown as solid circles. One atom of the basis is at the origin; the other atom is at $\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$, which means at the position $\mathbf{r} = \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$.

The hcp structure has the primitive cell of the hexagonal lattice, but with a basis of two atoms (Fig. 23). The fcc primitive cell has a basis of one atom (Fig. 13).

The ratio c/a (or a_3/a_1) for hexagonal closest-packing of spheres has the value $(\frac{8}{3})^{1/2} = 1.633$, as in Problem 3. It is usual to refer to crystals as hcp even if the actual c/a ratio departs somewhat from this theoretical value.

The number of nearest-neighbor atoms is 12 for both hcp and fcc structures. If the binding energy (or free energy) depended only on the number of

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.

H¹ 4K hcp 3.75 6.12	He⁴ 2K hcp 3.57 5.83
Li 78K bcc 3.491 3.59	Be hcp 2.27 3.59
Na 5K bcc 4.225	Mg hcp 3.21 5.21
K 5K bcc 5.225	Ca fcc 5.58
Rb 5K bcc 5.585	Sr fcc 6.08
Cs 5K bcc 6.045	Ba bcc 5.02
Fr —	Ra —
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
Sb rhomb.	Te hex. chains
Sn (α) diamond 6.49	In tetr. 3.25 4.95
Cd hcp 2.98 5.62	Ag fcc 4.09
Pd fcc 3.89	Pt fcc 3.92
Rh fcc 3.80	Ir fcc 3.84
Ru hcp 2.71 4.28	Os hcp 2.74 4.32
Tc hcp 2.74 4.40	Re hcp 2.76 4.46
Nb bcc 3.30	Ta bcc 3.30
Zr hcp 3.23 5.15	Hf hcp 3.19 5.05
Y hcp 3.65 5.73	La hex. 3.77 ABAC
Ce fcc 5.16	Pr hex. 3.67 ABAC
Th fcc 5.08	Pa tetr. 3.92 3.24
U complex	Np complex
Pu complex	Am hex. 3.64 ABAC
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
No —	Lr —
Md —	Fm —
Es —	Cf —
Bk —	Cm —
Ba —	At —
Po sc 3.34	Rn —
Bi rhomb.	Pb fcc 4.95
Tl hcp 3.46 5.52	Pb fcc 4.95
Hg rhomb.	Pb fcc 4.95
Au fcc 4.08	Pb fcc 4.95
Pt fcc 3.92	Pb fcc 4.95
Ir fcc 3.84	Pb fcc 4.95
Os hcp 2.74 4.32	Pb fcc 4.95
Re hcp 2.76 4.46	Pb fcc 4.95
Ta bcc 3.30	Pb fcc 4.95
Hf hcp 3.19 5.05	Pb fcc 4.95
La hex. 3.77 ABAC	Pb fcc 4.95
Ac fcc 5.31	Pb fcc 4.95
Ra —	Pb fcc 4.95
Fr —	Pb fcc 4.95