The Crystalline Form of Solids

Up to this point we have focused on generic properties of solids through thermodynamics, elasticity, the atomic and particle picture, and classical and quantum statistical mechanics – none of which require any special microscopic *morphology*, or three-dimensional form, of the solid. We have followed roughly the same path as the historical development of solid-state through the 19th century. And it was, indeed, a very productive century with impact made by solid state on nearly every branch of science and engineering: the understanding and purification of metals (particularly the "noble" metals: copper, silver and gold) as excellent conductors in electrical wires, circuits, motors; etc.; (2) the advancement of alloying to produce high stiffness (Young's modulus) and high yield strength materials such as steel (94% iron, 6% carbon); and (3) the discovery of fascinating and useful cross-field effects such as piezoelectricity (Pierre Currie), ferroelectricity, and pyroelectricity (all to be addressed later in the quarter). Most of these great developments were made with polycrystalline solids and remarkably most of them have stood the test of time.

Two developments occurred early in the 20th century that shifted the emphasis to crystals – solids having some degree of three-dimensional *translational and rotational symmetry*. These special type of symmetries mean that the if one could make an observation of some microscopic property the level of an atom, then they would get the same measurement result if they were to translate inside the solid by some length scale. This length scale, called the lattice constant, can and should depend on angular orientation. So the first task of crystal theory is to explain the translational symmetry and then explain its relation to rotational symmetry. The combination provides an elegant simplification to the microscopic mechanics and macroscopic analysis in many solid-state engineering problems.

The Crystal Lattice

In general a crystal is a collection of atoms whose time-average location in space lie on a lattice. A lattice is a mathematical construction consisting of a distribution of points in space, any of which can be reached from the others by a linear translation through *lattice vectors*. This general definition allows for a countless number of lattices. But in nature, and mathematically, the number is reduced to a special set of fundamental, *Bravais* lattices, by a secondary requirement that the *crystal appear identical after the translation is made*. There are thus two aspects to the definition of a Bravais lattice, one conceptual and one mathematical:

(1) A Bravais lattice is an inifinte array of points with a spatial arrangement and an angular orientation that both appear exactly the same no matter which lattice point is chosen.

(2) A Bravais lattice is the collection of vectors with respect to an arbitrary atom chosen as the origin for which

$$\mathbf{R} = l\,\mathbf{a}_1 + m\,\mathbf{a}_2 + n\,\mathbf{a}_3,$$

where $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ are any three "primitive" vectors not in the same plane and l, m, and n take on all integral values. It turns out that the two definitions are equivalent.

Examples of common Bravais lattices and their primitive vectors expressed in Cartesian coordinates:

(1) Simple cubic $\mathbf{a}_1 = a\mathbf{x}$; $\mathbf{a}_2 = a\mathbf{y}$; $\mathbf{a}_3 = a\mathbf{z}$

(2) Face-centered cubic:

$$\mathbf{a}_1 = (a/2)(\mathbf{y} + \mathbf{z}) \; ; \; \mathbf{a}_2 = (a/2)(\mathbf{z} + \mathbf{x}) \; ; \; \mathbf{a}_3 = (a/2)(\mathbf{x} + \mathbf{y})$$

(3) Body centered cubic: $\mathbf{a}_1 = a\mathbf{x}$; $\mathbf{a}_2 = a\mathbf{y}$ $\mathbf{a}_3 = (a/2)(\mathbf{x} + \mathbf{y} + \mathbf{z})$

Or a symmetric set: $\mathbf{a}_1 = (a/2)(\mathbf{y} + \mathbf{z} - \mathbf{x})$; $\mathbf{a}_2 = (a/2)(\mathbf{z} + \mathbf{x} - \mathbf{y})$; $\mathbf{a}_3 = (a/2)(\mathbf{x} + \mathbf{y} - \mathbf{z})$

Or other possible sets too…

In fact there are a countless number of different primitive lattice vector...

- Primitive cell is the geometrical volume "spanned" by the chosen primitive vectors. When associated with primitive lattice vectors and translated through space, the primitive cells just fill all of the crystal space with *no overlap and no voids*.
- The conventional unit cell reflects the space group of the crystal. For example, all cubic crystals are defined by a conventional cell that is, of course larger than the primitive cell except for simple cubic.

14 Bravais Lattices

What makes Bravais lattices so special (and few in number) is the their combination of translational and rotational symmetry. In classifying the Bravais lattices (as done below), the first distinguishing factor is the rotational symmetry (often expressed by the 3-dim solid object having the same symmetry about its "major" axis). The second distinguishing factor relates to the translational symmetry.

Table I. Rotational and translational specification for 14 Bravais lattices

Rotation	Translation	# Elements
Cubic	(1) Simple; (2) Body centered; (3) Face centered	3 9 16
Tetragonal	(1) Simple; (2) Centered	2
Orthorhombic	(1) Simple; (2) Base centered; (3) Body centered, (4) Face centered	0
Monoclinic	(1) Simple; (2) Centered	0
Triclinic	Triclinic	0
Trigonal	Rhombohedral	4
Hexagonal	Simple	6

Many of the elemental solids crystallize in a pure Bravais lattice as listed in Table I, taken from Table 3 of Kittel Chapter 1 taking only those materials known to be solids at room temperature and known to crystallize in non-"complex" form. The fcc is the most common by far followed by bcc and simple hexagonal. We will get back to the fcc in awhile.

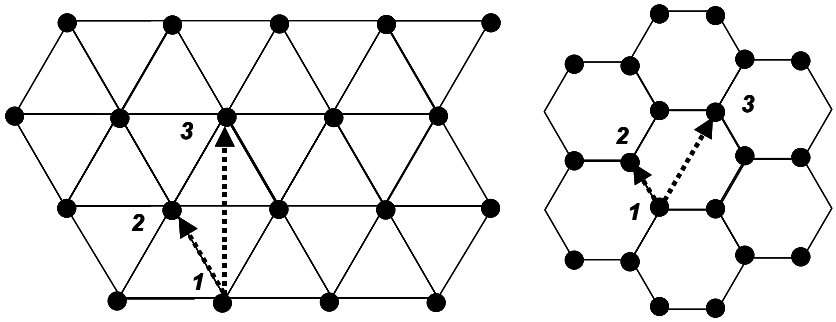

Fig. 1. (Left) triangular Lattice (a two-dim Bravais lattice). (Right) honeycomb Lattice (not a Bravais lattice). Translating from atom 1 to atoms 2 or 3 leads to the same appearance in the triangular lattice, but not for the honeycomb lattice.

Lattice with a Basis

Most natural and even many artificial (i.e., human made) crystals violate the defining requirements of a Bravais lattice. The solid does not appear identical as one moves from atom to atom either because of orientational changes (e.g., a rotation is required to get back to the same appearance), or because of chemical changes (two or more different atomic species make up the crystal). The first "orientational" violation is displayed nicely in the examples given in Fig. 1 for a two-dimensional triangular (Bravais) lattice vs a the two-dim honeycomb (non-Bravais) lattice. A good three-dim example is the diamond crystal structure behind silicon.

The second "chemical" violation occurs in most naturally occurring crystals because they are *compounds* (i.e., materials having two or more atomic species). And in many materials, both requirements are violated. A good example is the popular "zincblende" crystal structure behind the popular compound semiconductors GaAs and InP. A number of commonly occurring (whether natural or syntethic) non-Bravais crystal structures is given in Table II, not necessarily listed in order of importance.

A remarkable fact is that the majority of these non-Bravais crystal structures have an embedded Bravais lattice such that the other atoms, having the same speciation or not, can be thought of as "satellites.". Then the primitive unit cell associated with each Bravais lattice site can be thought of as having a "basis" – the arrangement of *all* the atoms within the cell. The entire crystal is then constructed by putting together these primitive cells contiguously as before. The "repeat unit" is the primitive cell. The satellite atoms "go along for the ride".

Table II. Common and Important Non-Bravais Crystal Structures

Crystal Structure	Embedded Bravais	Basis	Number of Elements
Diamond	fcc	Two interpenetrating fcc ¼-way along unit-cube body diagonal	4
Hexagonal close packed (hcp)	Hexagonal	Two interpenetrating simple hexagonal; "cannonball" stacked	22

NaCl (rocksalt)	fcc	Two interpenetrating fcc ½-way along unit-cube side	NA
CsCl	Simple Cubic	Two interpenetrating sc ½-way along unit-cube body diagonal	NA
Zincblende	fcc	Same as diamond but different atomic species on two interpenetrating fcc's	NA
Wurtzite	Hexagonal	Same as hcp but different atomic species on two interpenetrating SH	NA

Also shown in the Table is the number of elements that crystallize with the given structure, again collected from Table 3 of Kittel Chap. 1. Note how common the hcp structure is, having 22 elements known to display this form of crystallinity at room temperature ! Part of the reason for this, and the commonality of the fcc elemental crystals, is the energetics of bonding explained qualitatively in the next paragraph.

Close Packing

Suppose we start with the triangular two-dim lattice of Fig. 1 and stack another triangular layer on top. If the second layer is stacked directly over the top, we get the simple hexagonal lattice of Table I. But there is another way to stack which leaves the second-layer atoms closer to the atoms in the first layer. This is the close-packed stacking, which can be done two possible ways as shown in Figs. 2(a) and (b). In both cases, the atoms in the second layer "fall" into the depression at the center of the triangle formed by three adjacent atoms in the bottom layer. It is exactly like stacking cannonballs (familiar to those students who might have visited a 19^{th} century fortress), or marbles, which naturally fall into the depression in the layer below because of gravity. And it would appear to be more favorable energetically for the atomic case too, not because of gravity but rather the covalent bonding phenomenology discussed earlier.

Now when the third layer is stacked on the second, there are two more possibilities. The atoms of the third layer can fall in the depressions of the second directly above the first layer. If the fourth layer is then directly over the second, this stacking sequence is repeated, we get the close-packed crystal. But the atoms in the third layer can fall in the other possible depression of the second layer, which is not directly over the atoms of the first layer. If the fourth layer is then placed directly over the first layer, the fifth over the second, and the sixth over the third, and this stacking sequence is repeated, we get the fcc structure with the stacking direction coinciding with the body diagonal of the conventional unit cube !

Judging from the commonality of the fcc and hcp structures, at least for the elements of Tables I and II, nature favors the close-packing configurations.

Polytypism

Because of the two possible ways of close-pack stacking a two-dim triangular lattice on top of another two-dim triangular lattice, one can represent the relative stacking orientation of the layers by three letters, conventionally done as A,B, and C. With this symbolism, an hcp crystal is represented by ABABAB…with "repeat unit" AB. And an fcc is represented by ABCABC… with repeat unit ABC. So by deduction, it should be possible to construct an infinite number of possible permutations with ever increasing repeat units; e.g.,

ABCACBABCACB…with repeat unit ABCACB….Such permutations are called "polytypes" and they are not just mathematical possibilities. Silicon carbide – one of the most important "wide-bandgap" semiconductors today is a hexagonal (Wurtzitic) crystal that displays over 45 different polytype forms (although only a few are commonly used in engineering devices).

Coordination number.

Associated with all the common crystal types is another important property called the coordination number. It is simply the number of nearest neighbors. An important metric for all Bravais lattices is the number of nearest neighbors around any given lattice point. A few values are listed below for the cubic crystal types. The fcc is the most "crowded" lattice of all four with 12 nearest neighbors. As one might expect, the coordination number is correlated to the mass density of these crystals, assuming the bond lengths are approximately fixed. This jibes with the elements in the periodic lattice too, as exemplified by the contrast between (fcc) crystalline Au with $\rho = 19.3 \times 10^3$ KG/m^3 , and (diamond) crystalline silicon with $\rho = 2.3 \times 10^3$ KG/m^3

Cubic crystal type	Coordination Number	
fcc	12	▲
bcc	8	|
sc	6	increasing packing efficiency
diamond cubic	4	|

As we shall see later in the coverage of electronic band structure, the packing density also correlates with electrical behavior: *cubic crystals of high packing fraction tend to be metallic, and those with low packing fraction tend to be insulators*.

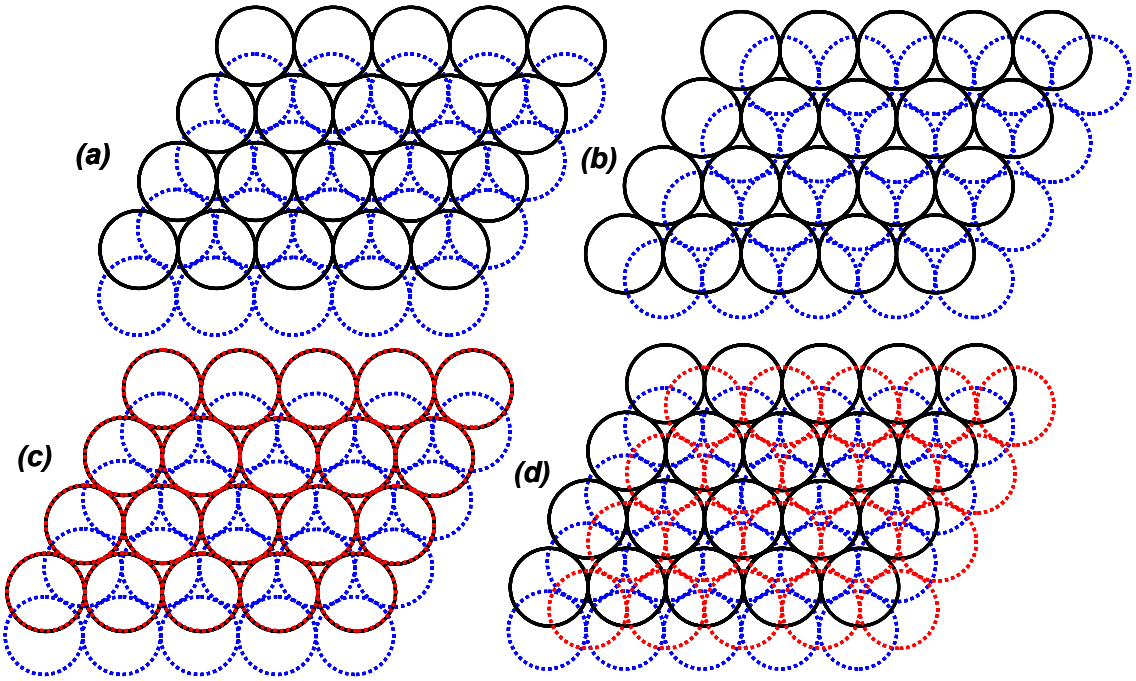

Fig. 2. Top view of close-packed stacking of triangular lattices: (a), (b) two equivalent ways of stacking the first two layers, [first layer is black; second layer is blue]; (c) stacking the third layer [red] on (a) so it is directly over the first layer (hexagonal close packing, or hcp); (d) stacking the third [red] on (a) so it is in the other possible choice close-packing arrangement of (b) (forming fcc lattice along cube body diagonal).

Wigner-Seitz Primitive Cell

With the multiplicity of ways of choosing Bravais lattice vectors, and the associated shape of the primitive cells, it useful (and geometrically inspiring) to choose a cell having the same symmetry as the point group (rotational symmetry) of the crystal. The most popular such cell is the Wigner-Seitz cell, and the recipe to construct it goes as follows: pick a lattice point and draw lines to all other atoms in the Bravais lattice. Then draw perpendicular planes through each line at the half-way point (perpendicular bisector planes). The smallest possible volume formed by all these planes is the Wigner-Seitz cell.

Wigner Seitz cells are difficult to draw in three dimensions. But a good example of their construction procedure and the resulting symmetry is given in Fig. 3 for the two-dimensional triangular lattice. The construction procedure still works except that the bisecting objects are lines, not planes. We start with the center atom and draw the lines to the nearest neighbors. The perpendicular bisecting lines just to the nearest neighbors clearly form the smallest possible enclosed volume, so the Wigner-Seitz cell becomes a perfect hexagon. And this reflects the "six-fold" symmetry of both the two-dim triangular lattice and the simple hexagonal lattice when the triangular lattices are stacked vertically on top of each other [note: a mistake made by some students is to think that a triangular lattice has three-fold "triangular" symmetry. But this pertains to rotation about the center of the triangle, and the *symmetry operations of Bravais lattices are always with respect to lattice points*]

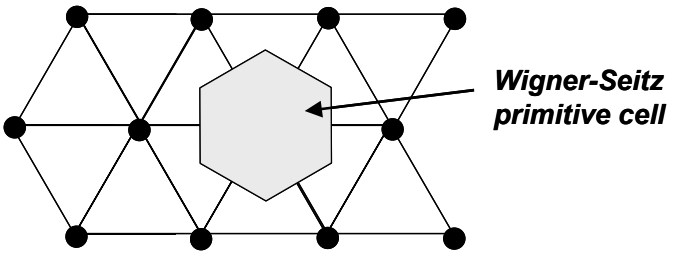

Fig. 3. Construction of Wigner-Seitz primitive cell from two-dimensional lattice

Lattice Sums: Cohesive Energy of Ionic Solids

Among many other things, the crystalline form of a solid makes it very easy to compute many physical quantities, such the cohesive energy. We will only do this for the ionic case, although the covalent case is similar. Recalling our model form of the ionic potential:

- We must sum the pair potential $\lambda \exp(-r/\rho) \pm \frac{q^2}{4\pi\varepsilon_0 r_0}$ over all ion pairs in the solid, keeping track of sign differences and distance between atoms
- First focus on a given ion and sum over all other ions.

Define:

R_{ij} = distance between i and j ions

$R_{ij} \equiv p_{ij} \bullet R$ where R is nearest neighbor separation

$p_{ij} \rightarrow$ real, positive number (not necessarily an integer !)

- Assume nuclear repulsive potential is important only between nearest neighbors. Define Z = number of nearest neighbors. (coordination number)

then $\phi_i = \sum_{j \neq i} \left(\lambda \exp\left(\frac{-r_{ij}}{\rho} + /- \frac{q^2}{4\pi\varepsilon_0 p_{ij} R} \right) \right) \equiv \sum_{j \neq i} \phi_{ij}$

$$\equiv Z\lambda e^{-R/\rho} - \frac{\alpha q^2}{4\pi\varepsilon_0 R}$$

(Note: Recall our convention for the ion polarity operator +/- : the first sign corresponds to having the charges in the ion pair the same; the second sign is when they are different. We choose the minus before the Coulomb term since we *want α to be positive*, and everything else in this term is positive. But the overall term has to be negative to get a stable potential; see discussion of ionic bond earlier in the notes).

Because of the addition of the negative sign on the Coulomb, we have to negate the +/- operator, so that $\alpha = \sum_{j \neq i} \frac{-/+}{p_{ij}} \rightarrow$ Madelung constant; for example: $p_{12} = 1$

and $\phi_i \equiv Z\lambda e^{-R/\rho} - \dfrac{\alpha q^2}{4\pi\varepsilon_0 R}$, which can provide a stable bonding length R_0 where $\left.\dfrac{d\phi}{dR}\right|_{R=R_0} = 0$.

• To get total solid cohesive energy, we must sum over all ions from i = 1 to N (N → number of ions)

$$\phi_0 = \sum_{i=1}^{N} \phi_i$$

But we cannot include all terms in $\sum_i$ because some are redundant (i.e., ϕ_{ij} and ϕ_{ji} correspond to the same pair-potential)

To see the summing process graphically we think of i and j indices as spanning a matrix (square)

$$i\downarrow \begin{pmatrix} \phi_{11} & \phi_{12} & \phi_{13} & \cdots & \phi_{1N} \\ \phi_{21} & \phi_{22} & \phi_{23} & \cdots & \phi_{2N} \\ & & & & \\ \phi_{N1} & \phi_{N2} & \phi_{N3} & \cdots & \phi_{NN} \end{pmatrix}$$
$$\rightarrow j$$

• Since we are dealing with pair potentials, the diagonal elements do not get counted. And the matrix is symmetric $\phi_{ij} = \phi_{ji}$, the same pair potential

• *Thus we only need to count half* of the off-diagonal elements, either upper or lower.

Mathematically this restricted set is given by $\dfrac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N}$ or $\dfrac{1}{2}\sum_{j}^{N}\sum_{i\neq j}^{N}$

But we already know $\sum_{j\neq i}\phi_{ij} = \phi_i \equiv Z\lambda e^{-R/\rho} - \dfrac{\alpha q^2}{4\pi\varepsilon_0 R}$

so $$\phi = \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N}\phi_{ij} = \frac{1}{2}\sum_{i=1}^{N}\phi_i$$

$$\phi = \frac{N}{2}\left(Z\lambda e^{-R/\rho} - \frac{\alpha q^2}{4\pi\varepsilon_0 R}\right)$$

As in pair potential analysis, we know this can have two values of R that result in $\left.\dfrac{d\phi}{dR}\right|_{R=R_0} = 0$

$$\frac{d\phi}{dR} = \frac{N}{2}\left(\frac{-Z\lambda}{\rho}e^{-R/\rho} + \frac{\alpha q^2}{4\pi\varepsilon_0 R^2}\right) = 0 \rightarrow Z\lambda = \frac{\rho\alpha q^2}{4\pi\varepsilon_0 R_0^2}\exp\left(R_0/\rho\right)$$

and $\phi_0 \equiv \phi(R = R_0) = \dfrac{N}{2}\dfrac{q^2\alpha}{4\pi\varepsilon_0 R_0}\left(\dfrac{\rho}{R_0} - 1\right)$, $R_0 \rightarrow$ stable nearest neighbor separation

The elegance of the lattice summing technique is that the resulting Madelung constant has the same value for *every solid* of the given (non-Bravais) crystal structure. For example,

Crystal Structure	α
Zincblende	1.6381
Sodium Chloride	1.74756

and this is one of the few times that 5 or 6 significant figures makes sense in engineering. It is a reflection of just how precise an ideal crystal lattice is.

And the nuclear repulsive parameters, λ and ρ, depend only on the atoms of the ion pair. For example Potassium and Chlorine, K and Cl, will have approximately the same λ and ρ for all crystal structures that KCl occurs in. But α will change between the structures (as will Z). So R_0 and ϕ_0 will change too. Once of the exercises in the HW addresses these facts. Note: to find R_0 one must do stability (derivative) analysis (or just pick the larger of two R_0s).

The Reciprocal Lattice: A Logical Consequence of Fourier's Theorem

Obviously if a solid is a perfect crystal, then many fundamental physical properties, such as the mass density and the total electron probability density, will have the same translational symmetry as the Bravais lattice. Perhaps less obvious is that the interaction of the crystal with external forces – the primary theme of the course – will also reflect the symmetry. In other words, the crystal properties become *periodic.* From one of the most powerful theorems in applied mathematics, we expect periodic functions to be reprsentable by a Fourier series.

As a reminder Fouriers theorem states that for a bounded function f(x) that is also periodic such that f(x) = f(x + L), then one can write:

$$f(x) = a_0 + \sum_{n=1}^{\infty} \{a_n \exp[j2n\pi x / L] + b_n \exp[-j2n\pi x / L]\} \equiv a_0 + \sum_{n=1}^{\infty} \{a_n \exp[jk_x x] + b_n \exp[-jk_x x]\}$$

where $k_x = 2\pi n/L$ is the circular *spatial* frequency

We can generalize this to a function periodic on the lattice by the

$$f(\vec{r}) = a_0 + \sum_{n=1}^{\infty} \{a_n \exp[j\vec{K} \cdot \vec{r}] + b_n \exp[-j\vec{K} \cdot \vec{r}]\}$$

We can now apply the periodic requirement that $f(\vec{r}) = f(\vec{r} + \vec{R})$ where $\vec{R}$ is any Bravais lattice vector. This leads to the results

$$f(\vec{r}) = a_0 + \sum_{n=1}^{\infty} \{a_n \exp[j\vec{K} \cdot (\vec{r} + \vec{R})] + b_n \exp[-j\vec{K} \cdot (\vec{r} + \vec{R})]\}$$

which can be true, in general, if and only if $e^{j\vec{K} \cdot \vec{R}} = e^{-j\vec{K} \cdot \vec{R}} = 1$

This, in turn requires

$$\vec{K}\cdot\vec{R} = 2\pi n \quad \text{, n = integer} \qquad (*)$$

The $\vec{K}$ s are the circular spatial frequencies of the Fourier series, better known (in solid-state physics) *as the reciprocal lattice vectors*.

Equation (*) becomes the definitive expression for constructing the reciprocal lattice vectors. Once obtained, they span the "Fourier space" of the given Bravais lattice, and because they are necessarily discrete, they too form a lattice – the "reciprocal lattice." It is important up front to realize that the $\vec{K}$ s must still ultimately be represented in the same Cartesian space as the $\vec{R}s$. They are just a different "basis set."

Perhaps the easiest way to construct the $\vec{K}$ s easily is to anticipate the fact that one can write $\vec{K} = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3$ and use $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$ to create a very simple inner product. We simply choose, $\vec{b}_1 \perp$ to $\vec{a}_2$ and $\vec{a}_3$ such that

$$\vec{b}_1\cdot\vec{R} = \text{integer} \times 2\pi$$

So that we get the well-known relations,

$$\vec{b}_1 = 2\pi\left[\frac{\vec{a}_2\times\vec{a}_3}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}\right]$$

$$\vec{b}_2 = 2\pi\left[\frac{\vec{a}_3\times\vec{a}_1}{\vec{a}_2(\vec{a}_3\times\vec{a}_1)}\right]$$

$$\vec{b}_3 = 2\pi\left[\frac{\vec{a}_1\times\vec{a}_2}{\vec{a}_3(\vec{a}_1\times\vec{a}_2)}\right]$$

We can show the "primitive" reciprocal lattice vectors – the $\vec{b}'s$ - have the correct properties. It's obvious $\vec{a}_i\cdot\vec{b}_j = 2\pi\delta_{ij}$ where $\delta_{ij} = 1$ if i = j ; = 0 if i ≠ j. It can be shown (a mathematical proof) that there is no other $\vec{K}'s$ that satisfy $e^{j\vec{K}\cdot\vec{R}} = 1$ or $e^{-j\vec{K}\cdot\vec{R}} = 1$ except linear combinations of the $\vec{K}'s$. If there was one, the coefficients would have to be non-integral $\Rightarrow$ an $\vec{R}$ could be found such that $e^{j\vec{K}\cdot\vec{R}} \neq 1$.

As an example we consider the fcc "direct lattice for which we have the symmetrical set of primitive lattice vectors

$$\vec{a}_1 = a/2\left(\hat{y}+\hat{z}\right)$$

$$\vec{a}_2 = a/2\left(\hat{z}+\hat{x}\right)$$

$$\vec{a}_3 = a/2\left(\hat{y}+\hat{x}\right)$$

Substitution into the above formula leads to

$$\vec{b}_1 = \frac{2\pi}{a^3/4}\times\left(\frac{a^2}{4}\right)\left[\left(\hat{z}+\hat{x}\right)+\left(\hat{y}+\hat{x}\right)\right] = \frac{2\pi}{a}\left[-\hat{x}+\hat{y}+\hat{z}\right]$$

volume of primitive cell

Continuing, we find

$$\vec{b}_2 = \frac{2\pi}{a}\left[\hat{x}-\hat{y}+\hat{z}\right]$$

$$\vec{b}_3 = \frac{2\pi}{a}\left[\hat{x}+\hat{y}-\hat{z}\right]$$

And these are just $4\pi/a^2$ times the "symmetrical" set of primitive lattice vectors for the bcc lattice defined on p. 2 of these notes. The "Fourier space" of a an fcc lattice is bcc lattice !

The Wigner-Seitz Cell of the Reciprocal Lattice: The Brillouin Zone

As in the direct crystal space, we can define a three dimensional "primitive" cell with respect to a chosen point by the same (Wigner-Seitz) perpendicular bisector recipe as for the direct lattice. And as in the direct lattice, if repeated through the solid by reciprocal lattice vectors, it will just fill all of reciprocal space with no voids or overlaps. For historical reasons, this "primitive" cell of reciprocal space is called the 1st Brillouin zone.

Directions in Space and Lattice Planes

Any three non-co-linear points define a plane $\rightarrow \infty$ # points in plane. It's not so obvious that for any plane, there is a family of planes parallel to the first one that contains points. Definition: a "family" of planes is formed by a given plane and all parallel planes which contain the points of a Bravais Lattice

Theorem: For every "family" of planes in real space, there exists a $\vec{K}$ vector in reciprocal space such that $\vec{K}$ is perpendicular to the planes. The smallest such $\vec{K}$ vector has length $\frac{2\pi}{d}$ where d is the spatial separation between planes.

Conversely, for every reciprocal lattice vector there is a corresponding plane in direct space. So if we write, $\vec{K} = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3$, we can conveniently use the coefficients m_1, m_2, and m_3 to uniquely represent the planes. The convention in crystallography is to use the following bracket notation

$$(m_1 , m_2 , m_3) \rightarrow \text{plane}$$

$$[m_1 , m_2 , m_3] \rightarrow \text{family of planes}$$

We will come back and develop more concepts and mathematics in reciprocal lattice space as the need arises: particularly in developing the interaction between mechanical waves and the lattice (phonons, when quantized), and the interaction between electron (de-Broglie) waves and the lattice (energy band structure).