

Physics 195 / Applied Physics 195 — Assignment #4

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Due: 12:45pm + 10 min grace period, Oct. 13, 2017 at the dropbox outside Maxwell-Dworkin Room 131.

Problem 1 (130 pt; no collaboration allowed): Two-dimensional (2D) lattices and crystals

(a) In two dimensions, there exist five kinds of Bravais lattices, which are shown in Fig. 1. Draw at least three primitive cells for each of the five lattices. Draw the Wigner-Seitz cell for each of the five lattices.

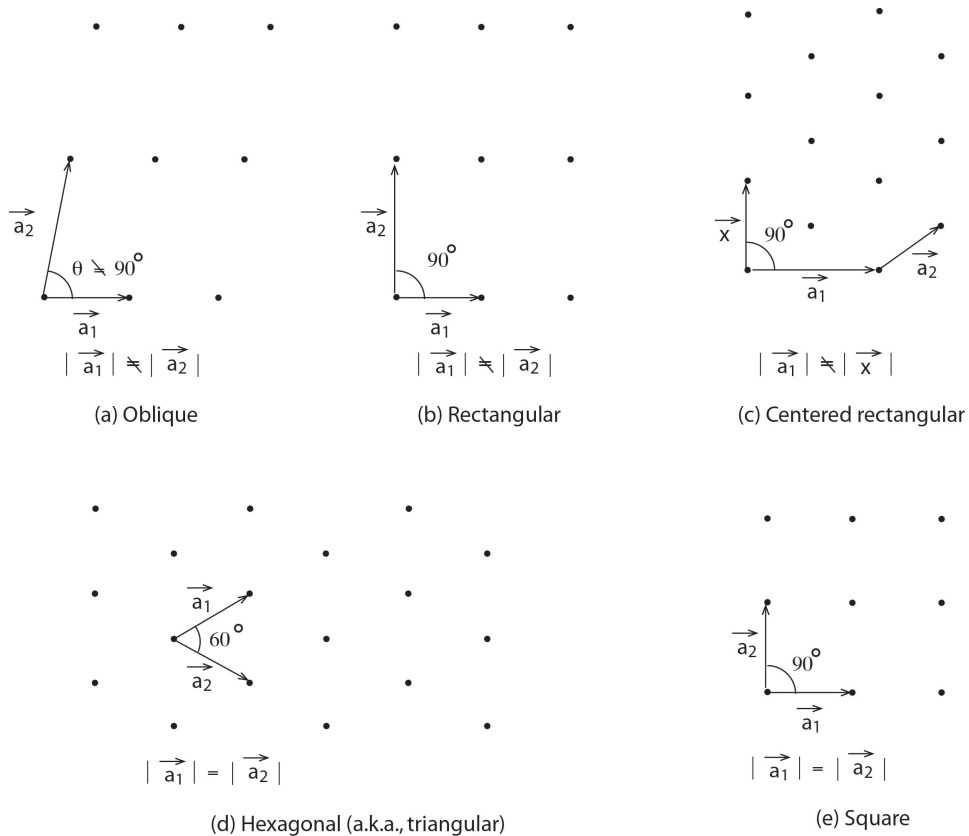


Figure 1: Five types of 2D Bravais lattices: (a) oblique lattice; (b) rectangular lattice; (c) centered rectangular lattice; (d) hexagonal lattice, also known as triangular lattice; (e) square lattice.

(b) The hexagonal lattice [Fig. 1(d)] is a special case of the centered rectangular lattice [Fig. 1(c)]. Find the ratio $|\vec{a}_1|/|\vec{x}|$ (here \vec{a}_1 and \vec{x} are in reference to Fig. 1(c)), for which the centered rectangular lattice becomes the hexagonal lattice.

(c) Let a 2D crystal be constructed by packing circles (representing atoms), with each circle centered at each hexagonal lattice point. Find the packing ratio—the ratio of the area occupied by the circles to the total area—for this 2D hexagonal lattice crystal. Repeat the calculation of the packing ratio for a 2D square lattice crystal. Which crystal packs more densely (and hence can be more energetically favorable)?

(d) Red dots of Fig. 2 are carbon atoms that form graphene, a one-atom thick monolayer of graphite. As discussed in Lecture #6, this honeycomb net of red dots (carbon atoms) is not a Bravais lattice, and hence graphene should be described with the lattice-with-a-basis formalism. We can use the hexagonal lattice (black dots of Fig. 2) spanned by the primitive lattice vectors \vec{a}_1 and \vec{a}_2 as the Bravais lattice in this case,

with the corresponding primitive unit cell containing two carbon atoms [Fig. 2].

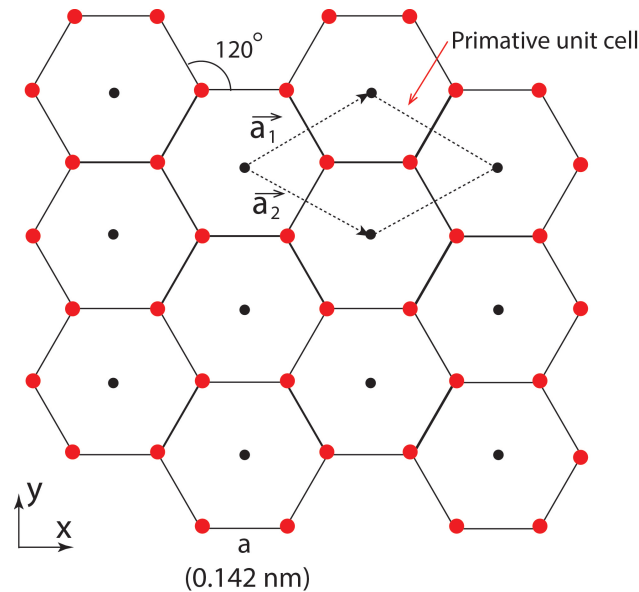


Figure 2: Honeycomb net of carbon atoms (red dots) in graphene. Black dots form a 2D hexagonal lattice, which we saw in Fig. 1(d).

- Show that \vec{a}_1 and \vec{a}_2 are given by:

$$\vec{a}_1 = \frac{3a}{2}\hat{x} + \frac{\sqrt{3}a}{2}\hat{y}; \quad (1)$$

$$\vec{a}_2 = \frac{3a}{2}\hat{x} - \frac{\sqrt{3}a}{2}\hat{y}, \quad (2)$$

where the length a is shown in Fig. 2. Complete the lattice-with-a-basis description of graphene by specifying the positions of the two carbon atoms in the primitive unit cell.

- Calculate the area of the primitive unit cell, A_{cell} .
- Express the primitive lattice vectors \vec{b}_1 and \vec{b}_2 of the reciprocal lattice, and identify the type of the reciprocal lattice (among the five 2D Bravais lattice choices). Draw the 1st Brillouin zone, specifying characteristic dimensions. Calculate the area of the Brillouin zone, A_{BZ} , and show that

$$A_{BZ} = \frac{(2\pi)^2}{A_{cell}}. \quad (3)$$

(e) Determine the reciprocal lattice of each type of the five 2D direct Bravais lattices (you have already done this for the hexagonal lattice in Part (d)). Check Eq. (3) holds true for each case.

Problem 2 (170 pt; no collaboration allowed): Three-dimensional (3D) lattices and crystals

(a) A 3D crystal is described by the direct lattice spanned by the following primitive lattice vectors

$$\begin{aligned} \vec{a}_1 &= 3\gamma\hat{x}; \\ \vec{a}_2 &= 3\gamma\hat{y}; \\ \vec{a}_3 &= 3\gamma/2(\hat{x} + \hat{y} + \hat{z}), \end{aligned} \quad (4)$$

where γ is a constant with the unit of length. Show that this is a BCC crystal. Calculate the volume of the conventional unit cell and primitive unit cell in terms of γ .

(b) Prove that the reciprocal lattice of FCC lattice is BCC, and the reciprocal lattice of BCC lattice is FCC.

(c) The crystal structure of iron is BCC at temperatures below 910°C and FCC above. Calculate the ratio of the mass densities of the two structures, assuming that the atoms are close packed spheres, whose diameters are the same in both structures. If the density of BCC iron is $7,900 \text{ kg/m}^3$, what is the lattice constant of the conventional unit cell?

(d) At about 13°C , gray tin ($\alpha\text{-Sn}$) undergoes a phase transition to white tin ($\beta\text{-Sn}$). $\alpha\text{-Sn}$ has a diamond structure with a conventional-unit-cell lattice constant of $a = 0.649 \text{ nm}$, while $\beta\text{-Sn}$ has a body-centered tetragonal structure with conventional-unit-cell lattice constants of $a = 0.583 \text{ nm}$ and $c = 0.318 \text{ nm}$. Calculate the mass densities in the two phases.

(e) Give a lattice-with-a-basis description for the barium titanate (BaTiO_3) crystal in Fig. 3.

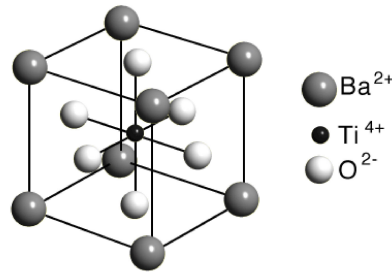


Figure 3: Barium titanate (BaTiO_3).

(f) Give a lattice-with-a-basis description for the gallium arsenide (GaAs) crystal in Fig. 4.

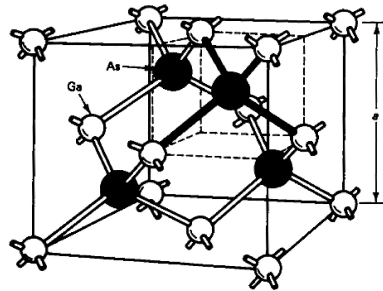


Figure 4: Gallium arsenide (GaAs).

(g) Consider a general 3D Bravais direct lattice with a primitive unit cell volume of V_{cell} . Prove the following general and very important relationship

$$V_{BZ} = \frac{(2\pi)^3}{V_{cell}} \quad (5)$$

where V_{BZ} is the volume of the 1st Brillouin zone.

(h) Prove that the density of lattice points per area in a lattice plane is d/V_{cell} , where d is the distance from this lattice plane to its neighboring parallel lattice plane and V_{cell} is as defined in Part (g). Subsequently, prove that in the FCC lattice, the lattice planes with the highest point densities per area are the $\{111\}$ planes where the Miller index is in reference to the conventional unit cell.

(i) Show that the reciprocal lattice of the reciprocal lattice is the direct lattice.

Problem 3 (0 pt): X-ray diffraction — This is a bonus problem, and will not be graded.

Let's recap on the derivation of the Laue condition (Lecture #7). Strength of light diffraction by a crystal is proportional to $|\langle \vec{k}' | n(\vec{r}) | \vec{k} \rangle|^2$, where $n(\vec{r})$ is the periodic electron density distribution across the crystal.¹ As $n(\vec{r} + \vec{R}) = n(\vec{r})$ for any direct lattice vector \vec{R} , $n(\vec{r}) = \sum_{\vec{G}} n_{\vec{G}} e^{i\vec{G} \cdot \vec{r}}$ where \vec{G} represents reciprocal lattice vectors with $n_{\vec{G}}$ being Fourier components. Then the overlap integral is

$$\langle \vec{k}' | n(\vec{r}) | \vec{k} \rangle = \int_{\text{crystal}} e^{-i\vec{k}' \cdot \vec{r}} n(\vec{r}) e^{i\vec{k} \cdot \vec{r}} d^3 \vec{r} = \sum_{\vec{G}} n_{\vec{G}} \int_{\text{crystal}} e^{i[\vec{G} - (\vec{k}' - \vec{k})] \cdot \vec{r}} d^3 \vec{r}. \quad (6)$$

This vanishes unless $\vec{k}' - \vec{k}$ is equal to a certain \vec{G} . Thus the Laue condition, $\vec{k}' - \vec{k} = \vec{G}$, is necessary for diffraction to occur. In contrast, it is in general not sufficient for diffraction to occur; even if $\vec{k}' - \vec{k} = \vec{G}$ for a certain \vec{G} , the resulting overlap integral

$$\langle \vec{k}' | n(\vec{r}) | \vec{k} \rangle = V n_{\vec{G}} = \int_{\text{crystal}} e^{-i\vec{G} \cdot \vec{r}} n(\vec{r}) d^3 \vec{r} \quad (7)$$

will vanish if $n_{\vec{G}} = 0$ (V : crystal volume). The situation of $n_{\vec{G}} = 0$ occurs, for example, if a monatomic crystal with BCC lattice is described using SC conventional unit cell with a basis (two identical atoms). The spatial frequency of $n(\vec{r})$ coming from all atoms can be twice larger—along certain crystal directions—than the spatial frequency described by \vec{G} vectors derived from the SC lattice that misses out body-centered atoms; therefore, $n_{\vec{G}} = 0$ for a certain set of \vec{G} vectors. For another example, for a diatomic crystal of CsCl structure, whose description is now natural with the SC lattice a basis (two different atoms), if the two basis atoms have similar electron density distributions, $n_{\vec{G}}$ can be close to zero for certain \vec{G} vectors for the same reason as above.

More generally, $n_{\vec{G}}$ will vary with the positions and electron density distributions of basis atoms. To show this explicitly, we first decompose $n(\vec{r})$ into $n(\vec{r}) = \sum_{i=1}^u n_i(\vec{r} - \vec{d}_i)$ (u : number of basis atoms per unit cell; n_i : periodic electron density distribution across the crystal due to the i -th basis atoms; \vec{d}_i : position of the i -th basis atom in each unit cell). By plugging this into Eq. (7), we obtain

$$\begin{aligned} \langle \vec{k}' | n(\vec{r}) | \vec{k} \rangle &= V n_{\vec{G}} = \sum_{i=1}^u \int_{\text{crystal}} e^{-i\vec{G} \cdot \vec{r}} n_i(\vec{r} - \vec{d}_i) d^3 \vec{r} = \sum_{i=1}^u \left[e^{-i\vec{G} \cdot \vec{d}_i} \times \int_{\text{crystal}} e^{-i\vec{G} \cdot \vec{r}} n_i(\vec{r}) d^3 \vec{r} \right] \\ &= \sum_{i=1}^u f_i e^{-i\vec{G} \cdot \vec{d}_i}, \end{aligned} \quad (8)$$

where

$$f_i \equiv \int_{\text{crystal}} e^{-i\vec{G} \cdot \vec{r}} n_i(\vec{r}) d^3 \vec{r}, \quad (9)$$

is the property of the i -th basis atom and is roughly proportional to Z_i , the atomic number. For $\vec{G} = l\vec{b}_1 + h\vec{b}_2 + k\vec{b}_3$ (l, h, k : integers) and $\vec{d}_i = x_i\vec{a}_1 + y_i\vec{a}_2 + z_i\vec{a}_3$ (x, y, z : real),

$$\langle \vec{k}' | n(\vec{r}) | \vec{k} \rangle = V n_{\vec{G}} = \sum_{i=1}^u f_i \exp[-i2\pi(lx_i + hy_i + kz_i)]. \quad (10)$$

¹Lecture #7 uses $V(\vec{r})$ —effective periodic potential for light scattering—in lieu of $n(\vec{r})$. $V(\vec{r}) \sim n(\vec{r})$ for light scattering.

This explicitly shows the impact of the electron density distribution and position of each basis atom on the diffraction strength.

- (a) Let a monatomic BCC crystal be described using the SC conventional unit cell with two basis atoms. Show that diffraction does not occur for $(l, h, k) = (1, 0, 0)$ but occurs for $(l, h, k) = (1, 0, 0) \times 2$; can you explain this from the Bragg point of view, considering relevant lattice planes? Show that diffraction occurs for both $(l, h, k) = (1, 1, 0)$ and $(l, h, k) = (1, 1, 0) \times 2$; can you again explain this from the Bragg point of view? Show in general that no diffraction occurs if $l + h + k$ is an odd integer.
- (b) Consider a monatomic FCC crystal described using the SC conventional unit cell with four basis atoms. Show that no diffraction occurs unless all of l , h , and k are even integers, or all of them are odd integers.
- (c) A monatomic crystal of diamond structure is described using the SC conventional unit cell with eight basis atoms. State the condition for l , h , and k for diffraction to occur.
- (d) Let a NaCl crystal be described with the SC conventional unit cell containing 8 basis atoms (4 sodium and 4 chloride atoms). Evaluate Eq. (10), while denoting the atomic form factor (f_i) for sodium as f_{Na} and that for chloride as f_{Cl} . You may use the approximation $f_{Cl}/f_{Na} \sim 17/11$. Show that diffraction occurs only when all of l , h , and k are even integers, or all of them are odd integers. Which of these two diffraction groups exhibits stronger diffraction?