Course C6: Answer Sheet 3

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Answer 1

The stereogram has four–fold symmetry so the $\{001\}$ poles of the cubic ceramic and silver coincide. The four–fold symmetry also indicates that the four poles in the middle could be of the form $\{110\}$ or $\{111\}$. This can be solved by calculating the angles of these forms with the $[001]_{\mathrm{Ag}}$ and $[001]_{\mathrm{ceramic}}$. Such calculations will show that the ones nearest the centre are $\{110\}_{\mathrm{ceramic}}$ (Fig. 1).

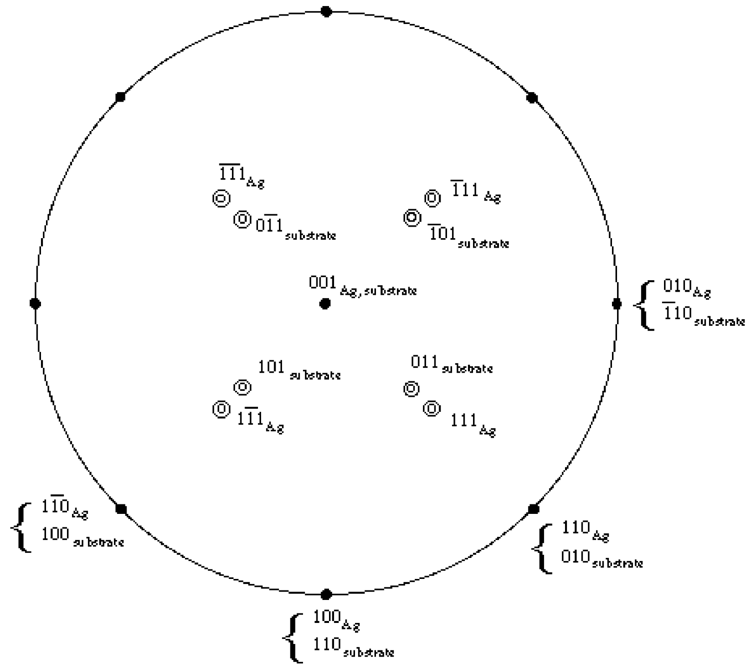

Figure 1: The orientation relationship is $(001)_{\mathrm{Ag}}||(001)_{\mathrm{ceramic}}$ and $[100]_{\mathrm{Ag}}||[110]_{\mathrm{ceramic}}$. This is because $a_{\mathrm{ceramic}} \simeq \sqrt{2}a_{\mathrm{Ag}}$, giving good lattice matching.

Answer 2

The Ewald sphere has a diameter which is the reciprocal of the wavelength of the radiation used. The direction of the incident beam is towards the origin of the reciprocal lattice. If any part of the sphere other than the origin lies on the surface of the sphere then the construction is such that it satisfies the Bragg law, as illustrated in Figure 2.

The Bragg law strictly applies to crystals which are infinitely large, since to cancel any deviant rays is then becomes possible to find another ray within the depth of the crystal which is exactly half a wavelength out of phase. Thus, only those at the Bragg angle are constructively interfered. When a crystal is made thin, it follows that it is not possible to find rays within the depth of the crystal which are exactly half a wavelength out of phase with deviant rays. Therefore, diffracted intensity is observed even when the exact Bragg condition is not satisfied.

In transmission electron microscopy, the sample is in the form of a thin foil. To account for the effect described above, the reciprocal lattice points in the Ewald construction are represented as spikes whose length (form) depends inversely on the thickness of the crystal, and which are normal to the plane of the foil. This makes it possible for the Ewald sphere to touch the spikes even though the Bragg condition is not satisfied. Put this together with the typically small wavelength of electrons (large diameter of the Ewald sphere) and the probability of detecting many spots on the pattern increases.

The sketch stereogram will show diads along $< 110 >$, triads along $< 111 >$ and tetrads along $< 100 >$ directions.

The normal to the electron diffraction pattern is clearly a two–fold axis and hence close to a $< 110 >$. Since all reciprocal lattice vectors on the pattern are normal to this, it can be deduced that the spots are as indexed in Figure 3. This can be done intuitively. Only two reciprocal lattice vectors need to be carefully deduced, the rest follow by linear combination of these two. Necessary to account for systematic absences associated with the body–centred cubic structure. Therefore worth checking the ratios of two reciprocal lattice vectors.

The intensities of the spots will vary for two reasons, their respective structure factors, and the location of the intersection of the Ewald sphere with the spikes – the intensities for a symmetrical pattern should for the latter reason decrease with distance from the origin of the pattern.

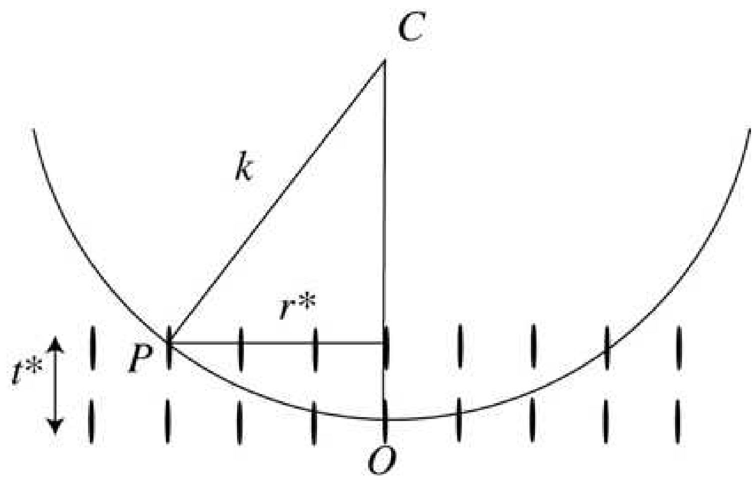

Figure 2: Ewald sphere construction.

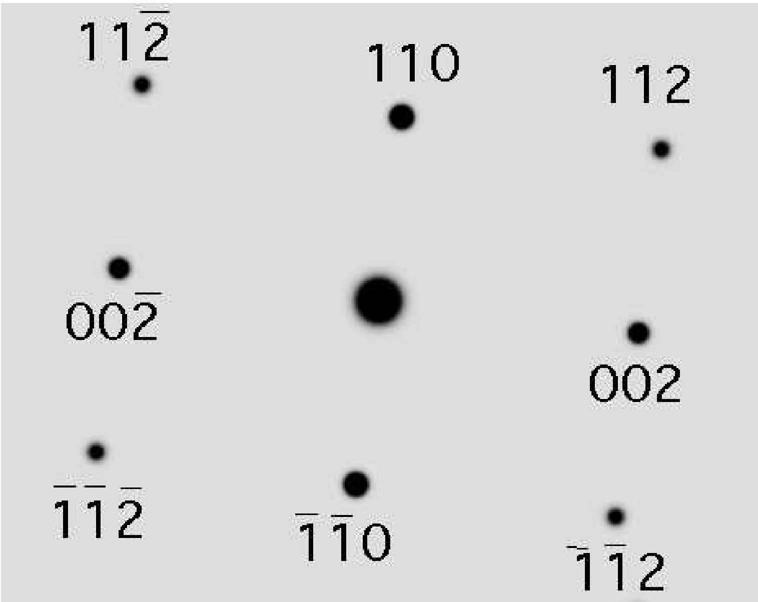

Figure 3: Labelled pattern.

Answer 3

The area of the polygon defined by a pair of vectors is given by the magnitude of the cross–product, i.e., $|\mathbf{a} \wedge \mathbf{b}|$, $|\mathbf{b} \wedge \mathbf{c}|$ and $|\mathbf{c} \wedge \mathbf{a}|$. The cross–product leads to a vector which is normal to the plane enclosed by the pair of vectors.

The volume is given by the area of the base multiplied by the height. When the base is considered to be defined by $\mathbf{a}$ and $\mathbf{b}$, the area is $|\mathbf{a} \wedge \mathbf{b}|$ and the height of the cell normal to the $\mathbf{a}$–$\mathbf{b}$ plane is

$$\mathbf{c}.\frac{\mathbf{a} \wedge \mathbf{b}}{|\mathbf{a} \wedge \mathbf{b}|} \tag{1}$$

If follows that the volume of the cell is

$$\mathbf{c}.\frac{\mathbf{a} \wedge \mathbf{b}}{|\mathbf{a} \wedge \mathbf{b}|} \times |\mathbf{a} \wedge \mathbf{b}| = \mathbf{c}.\mathbf{a} \wedge \mathbf{b} \tag{2}$$

Every vector in a reciprocal lattice defines a normal to a plane of the same indices as the components of the reciprocal lattice vector, and the vector has a magnitude which is the reciprocal of the spacing of those planes. Therefore, for each of the basis vectors,

$$\mathbf{c}^* = \frac{\mathbf{a} \wedge \mathbf{b}}{\mathbf{c}.\mathbf{a} \wedge \mathbf{b}} \qquad etc. \tag{3}$$

With this equation it is evident that $\mathbf{a}_i.\mathbf{a}^*{}_j = 0$ when $i \neq j$ and $\mathbf{a}_i.\mathbf{a}^*{}_j = 1$ when $i = j$. The angle between $\mathbf{a}$ and $\mathbf{b}^*$ is clearly 90°. Therefore, if a direction $[u\ v\ w]$ lies in a plane $(h\ k\ l)$,

$$[u\mathbf{a} + v\mathbf{b} + w\mathbf{c}].(h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*) = 0 = uh + vk + wl \tag{4}$$

Answer 4

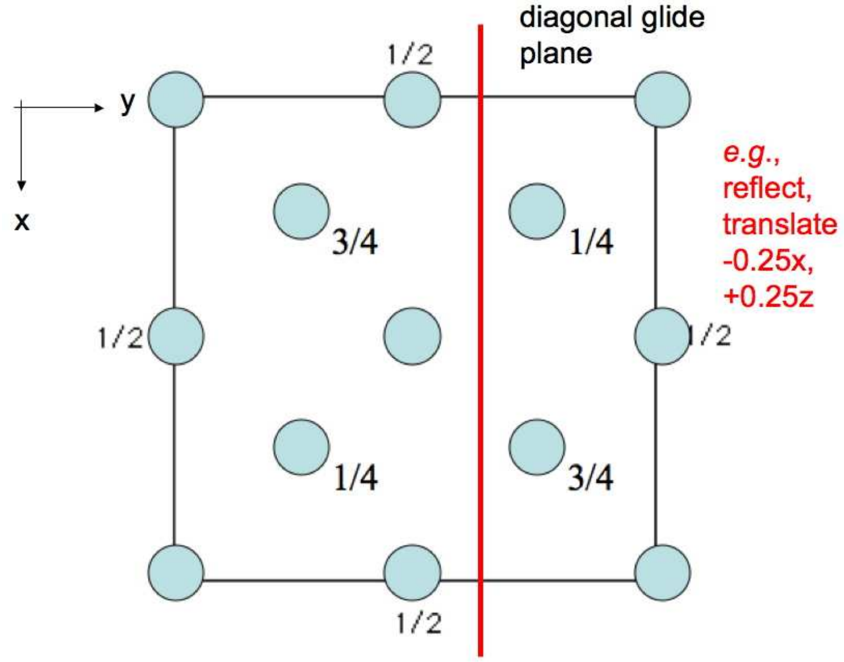

Figure 4: A diagonal glide plane in silicon. The shortest lattice vector is $\frac{a}{2} < 110 >$ and hence is the likely Burgers vector.

Answer 5

The central region surrounded by two annular rings occurs because of the intersection of the Ewald sphere first with the layer of the reciprocal lattice passing through its origin, and then with parallel layers located along $< 210 >$. The central regions of these latter layers do not intersect the Ewald sphere and hence appear as rings.

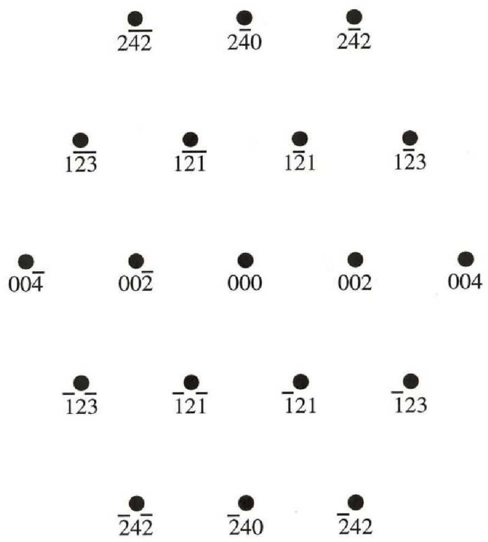

Figure 5: Indexing of the central zone. Note that once two spots are indexed, all the others can be generated by a linear combination of those two. After all, it only requires two vectors to specify a plane.

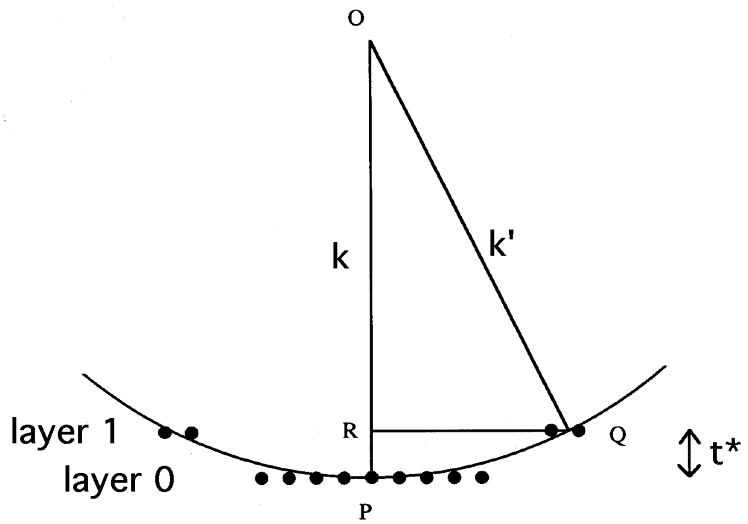

Figure 6: From Pythagoras, and given that QR$\equiv$ $\mathbf{r}*$, it follows that $\mathbf{r}^{*2} + (\mathbf{k} - \mathbf{t}^*)^2 = \mathbf{k}^2$. Given that $\mathbf{t}^*$ has a magnitude $1/t$, where t is the spacing of the planes normal to the [210] vector and that $\mathbf{k}$ has a magnitude $1/\lambda$, the required equation is obtained by rearranging the Pythagoras derivation.