SOLUTION 1

Exercise 1: Let d be the thickness of the silicon layer, A the total area of the modules, n the lifetime of the modules, η the average efficiency of the modules (taking into account temperature effects, cable losses,...) and $E_{inc,y}$ the annual incident irradiation.
The total annual produced energy by the modules (E_y) is then:

$$E_y = \eta \cdot E_{inc,y} \cdot A. \tag{1}$$

For a rough estimate of the area of the modules, we use:

$$V_{Si} = \frac{m_{Si}}{\rho_{Si}} = A \cdot d. \tag{2}$$

Thus,

$$A = \frac{m_{Si}}{\rho_{Si} \cdot d}. \tag{3}$$

We finally obtain the total energy for one gram silicon,

$$\begin{aligned} E_{tot,1\,g\,Si} &= \frac{\eta \cdot E_{inc,y} \cdot m_{Si} \cdot n}{\rho_{Si} \cdot d} \\ &= \frac{0.07 \cdot 2500\,\mathrm{kWh/m^2/y} \cdot 10^{-3}\,\mathrm{kg} \cdot 30\,\mathrm{y}}{2.3 \times 10^3\,\mathrm{kg\,m^{-3}} \cdot 200 \times 10^{-9}\,\mathrm{m}} \\ &\cong 11\,413\,\mathrm{kW\,h} \cong 4.1 \times 10^{10}\,\mathrm{J} \end{aligned}$$

The rest energy of 1 g Si is given by

$$E = m \cdot c^2 = 0.001\,\mathrm{kg} \cdot (3 \times 10^8\,\mathrm{m\,s^{-1}})^2 = 9 \times 10^{13}\,\mathrm{J} = 2.5 \times 10^7\,\mathrm{kW\,h}$$

Exercise 2:

a) Let a = 5.430 95 Å be the lattice parameter. With easy calculations, we get:

Neighboring atoms	Distances [Å]
quarter cube diagonal	$\frac{\sqrt{3}}{4}a = 2.35$
half face diagonal	$\frac{\sqrt{2}}{2}a = 3.84$
(1/4, 1/4, 1/4) to (1, 1/2, 1/2)	$\frac{\sqrt{11}}{4}a = 4.50$
cube face length	$a = 5.43095$
(0, 0, 0) to (3/4, 3/4, 1/4)	$\frac{\sqrt{19}}{4}a = 5.92$
(0, 0, 0) to (1, 1/2, 1/2)	$\sqrt{\frac{3}{2}}a = 6.65$
(1/4, 1/4, 1/4) to (1, 1, 1)	$\frac{3\sqrt{3}}{4}a = 7.06$
face diagonal	$\sqrt{2}a = 7.68$
cube diagonal	$\sqrt{3}a = 9.41$

Table 1: Distances between neighbors in a c-Si unit cell. The coordinates are normalized and the origin is on the lower left corner of the cube (for example (1/4, 1/4, 1/4) denotes the nearest neighbor of the atom on the origin that is shown on the figure).

The following peaks in the given experimental data correspond to distances beyond a single unit cell:

Neighboring atoms	Distances [Å]
(0, 0, 0) to (5/4, 3/4, -1/4)	$\frac{\sqrt{5}\sqrt{7}}{4}a = 8.03$
(0, 0, 0) to (3/2, 0, 1/2)	$\frac{\sqrt{5}\sqrt{2}}{2}a = 8.59$
(0, 0, 0) to (3/4, 3/4, 5/4)	$\frac{\sqrt{43}}{4}a = 8.90$
(0, 0, 0) to (5/4, 1/4, 5/4)	$\frac{\sqrt{51}}{4}a = 9.70$

Table 2: Some distances between neighbors in more than one unit cell.

b) The following relation holds for the angle β:

$$\sin\frac{\beta}{2} = \frac{\text{1/2 of the distance to the second next nearest neighbour}}{\text{distance to the nearest neighbour}}$$

leading to $\beta = 2\arcsin\left(\frac{\sqrt{2}a}{2\cdot 2}\cdot\frac{4}{\sqrt{3}a}\right) = 2\arcsin\left(\sqrt{\frac{2}{3}}\right) = 109.5°$.

c) As in the case of c-Si, the first peak at 2.35 Å is clearly visible. In the given reference[1], it is shown that the first bond length is the same (within 0.005 Å) for c-Si and a-Si.

The interpretation of the second-neighbor peak is less clear (unknown contribution of the third peak). The next peaks are not clearly resolved as well (broadening of the

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[1] K. Laaziri et al., Physical Review B **60** 19, 520-533 (1999)

peaks), indicating a major difference compared to c-Si. This can be understood in terms of small variations in β leading to deviation from the ideal network structure. Amorphous silicon has still a tetragonal (short-range) configuration, but no longer long-range order!

In this paper, it is also shown that vacancies are the major contribution to the smaller density of a-Si with respect to c-Si (the density of a-Si is about 2% less than the one of c-Si). In fact they find a coordination number (number of first next neighbours) of about 4 for c-Si, whereas the value for a-Si is slightly less (about 3.8-3.9).

Exercise 3 (Vacancies and voids in Si):

a) In each unit cell, there are 8 Si atom (see fig. 1: $8 \cdot \frac{1}{8} + 6 \cdot \frac{1}{2} + 4 \cdot 1$). The density ρ_V is then simply given by

$$\rho_V = \frac{\#\text{Si atoms}}{\text{volume}} = \frac{8}{a^3} \cong 5 \times 10^{22}\,\text{cm}^{-3}.$$

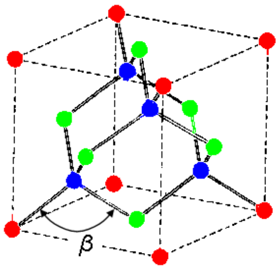

Figure 1: The colors highlight the different contribution of the atoms to the atomic density of a unit cell.

b) Here again, it is easier to work with the unit cell. On the (100) equivalent planes, each surface atom has 2 dangling bonds (DB) pointing out of the bulk, so two hydrogen atoms per atom, assuming full passivation (a hydrogen atom on each DB). However, with the help of fig. 2, on can see that there are 4 DB per unit cell on a (100) plane (The other 6 point out of the unit cell). This gives a surface density ρ_S of

$$\rho_S = \frac{\#\text{DB}}{\text{unit cell surface}} = \frac{4}{a^2} \cong 1.356 \times 10^{15}\,\text{cm}^{-2}.$$

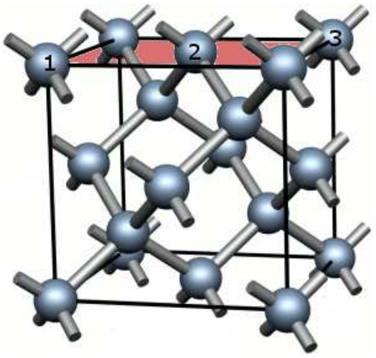

Figure 2: Only the atoms 1,2,3 contribute to DBs inside of a unit cell.

c) In first approximation and for an average value, the above density values within a sphere will be used, thus:

$$\#\mathrm{Si\,atoms} = \rho_\mathrm{V} \cdot \mathrm{V} = \rho_\mathrm{V} \cdot \frac{4}{3}\pi \mathrm{r}^3 \cong 8\,\mathrm{atoms}.$$

For the hydrogen, and using the rough approximation that each Si atom around the void has two hydrogen atoms, one gets:

$$\#\mathrm{H\,atoms} = \rho_\mathrm{S} \cdot \mathrm{S} = \rho_\mathrm{S} \cdot 4\pi \mathrm{r}^2 \cong 18\,\mathrm{atoms},$$

leading to $\delta \cong 0.44$.

For mono-, bi-, and trivacancies, this δ can be calculated exactly (see lecture). However, when getting experimental datas (e.g. void volume from SAXS expermients[2]), it is not trivial to find out the corresponding microscopic configuration.

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[2] Mahan et al., *Solar Cells* **27**, 465–476, 1989.