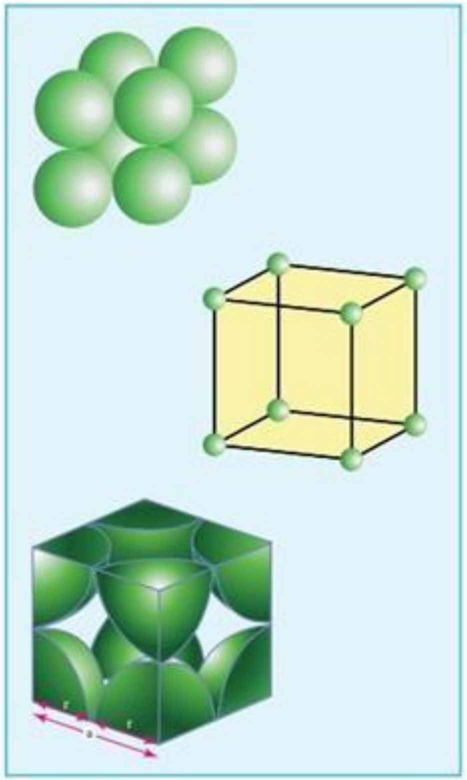
Module 1 Problems

Problem #1 : Find the APF for a simple cubic unit cell



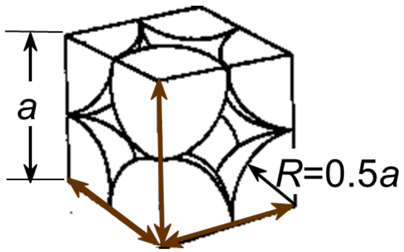
$$\therefore no\ of\ atoms\ in\ a\ SC\ unit\ cell = \left(\frac{Nc}{8}\right) = \left(\frac{8}{8}\right) = 1$$

Atomic Packing Factor (APF)

$$APF = \frac{\text{Volume of atoms in unit cell*}}{\text{Volume of unit cell}}$$

*assume hard spheres

- APF for a simple cubic structure = 0.52



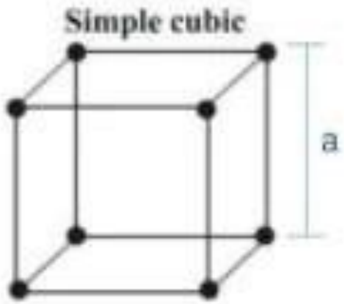
contains 8 x 1/8 =
1 atom/unit cell

$$APF = \frac{\underbrace{1}_{\frac{\text{atoms}}{\text{unit cell}}}\ \underbrace{\frac{4}{3}\pi(0.5a)^3}_{\frac{\text{volume}}{\text{atom}}}}{\underbrace{a^3}_{\frac{\text{volume}}{\text{unit cell}}}}$$

N_c is the number of atoms at the corners.

Primitive (or) simple cubic unit cell (SC)

Atomic Packing Factor for SC (Simple cubic)



Let a = lattice constant

r = atomic radius

The center of each atom coincides with the different corners of the cube and the atoms touch each other at their periphery.

Let us take a =2r

Each one of the atoms at the corners of the cube has effectively only 1/8th of its volume present inside the cubic cell,

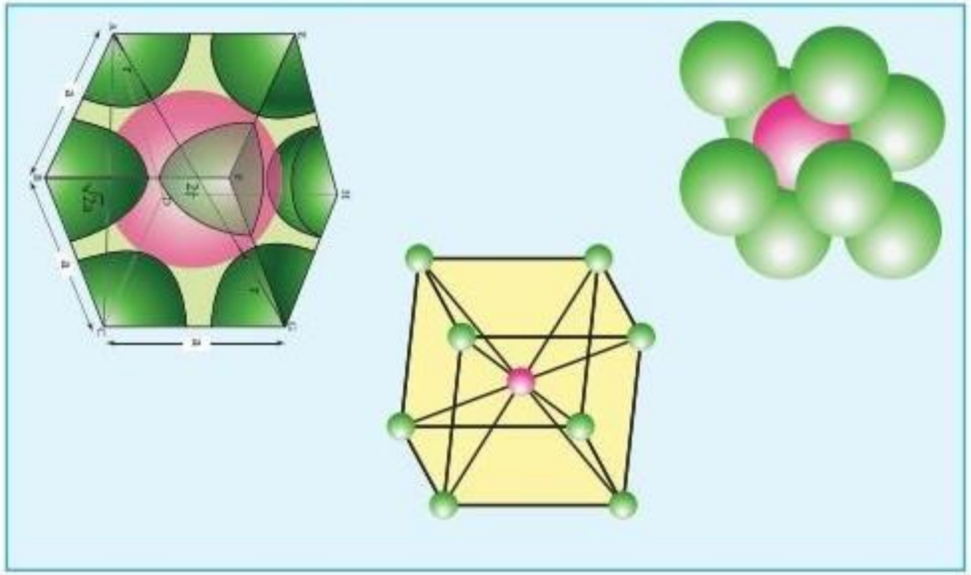
$$8\,X\,\frac{1}{8} = 1\ atoms$$

$$\frac{\text{Volume of atoms}}{\text{Volume of unit cell}} = \frac{\text{No. of atoms} \times \text{vol. of each atom}}{\text{Vol. of unit cell}}$$

$$\text{APF} = \frac{1 \times \frac{4\pi r^3}{3}}{a^3} = \frac{4\pi r^3}{3(2r)^3} \qquad \left[\begin{array}{l}\text{Since Vol. of sphere} = \frac{4\pi r^3}{3} \\ \text{and } a = 2r\end{array}\right]$$

APF = 0.52

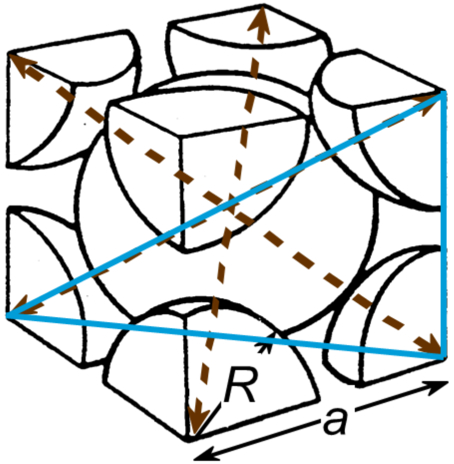
Problem #2: Find the APF for a Body – Centred Cubic unit cell (BCC)

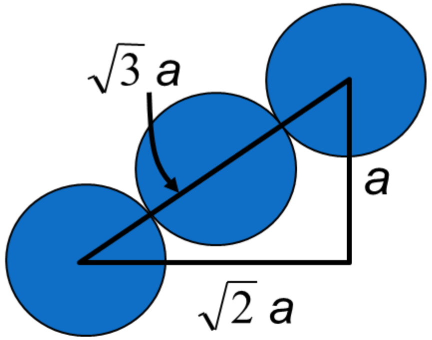


$$\therefore \text{Number of atoms in a bccunitcell} = \left(\frac{Nc}{8}\right) + \left(\frac{N_b}{1}\right)$$
$$= \left(\frac{8}{8} + \frac{1}{1}\right)$$
$$= (1+1)$$
$$= 2$$

Atomic Packing Factor: BCC

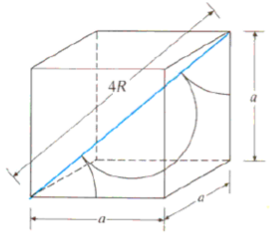
- APF for a body-centered cubic structure = 0.68





Close-packed directions:
length = $4R = \sqrt{3}\,a$

$$\text{APF} = \frac{\overbrace{2}^{\text{atoms/unit cell}} \; \overbrace{\frac{4}{3}\pi(\sqrt{3}a/4)^3}^{\text{volume/atom}}}{\underbrace{a^3}_{\text{volume/unit cell}}}$$

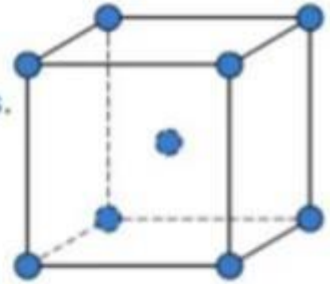


Body – Centred Cubic unit cell (BCC)

Atomic Packing Factor for BCC

Solution

There is one full atom at the center and one atom at each of the eight corners.



Therefore effective number of atoms inside each unit cell is,

$$1 + 8X\frac{1}{8} = 2\,atoms$$

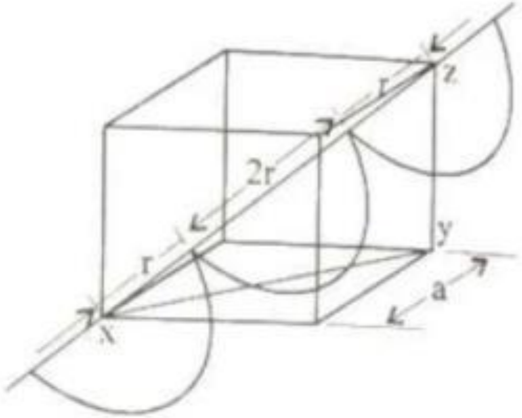
To find 'a' in terms of 'r'

$$xy = \sqrt{a^2 + a^2} = \sqrt{2}a \text{ (Solid diagonal)}$$

$$(xz)^2 = (4r)^2 = \left(\sqrt{2}a\right)^2 + a^2$$

$$4r = \sqrt{3a^2}$$

$$a = \frac{4r}{\sqrt{3}}$$

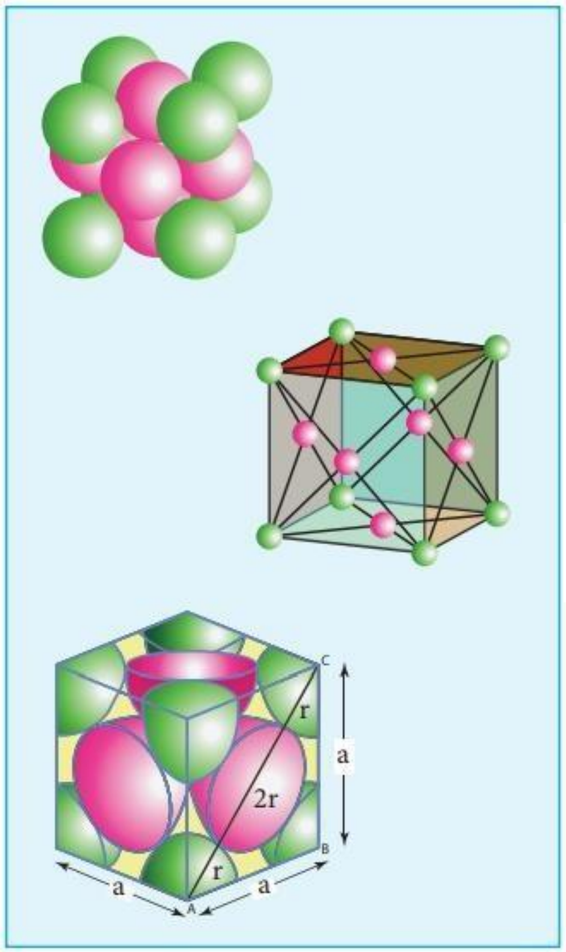


$$APF = \frac{\text{No. of atoms} \times \text{vol. of each atom}}{\text{vol. of unit cell}}$$

$$APF = \frac{2 \times \frac{4\pi r^3}{3}}{a^3} = \frac{2 \times 4\pi r^3}{3\left(\frac{4r}{\sqrt{3}}\right)^3}$$

$$\mathbf{APF = 0.68}$$

Problem #3: Find the APF for a Face – Centred Cubic unit cell (FCC)



$$\therefore \text{Number of atoms in a fcc unitcell} = \left(\frac{N_c}{8}\right) + \left(\frac{N_f}{2}\right)$$

$$= \left(\frac{8}{8} + \frac{6}{2}\right)$$

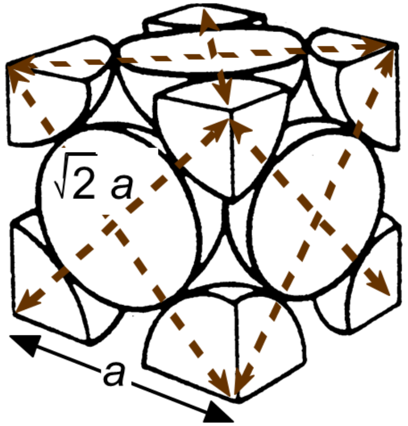
$$= (1+3)$$

$$= 4$$

Atomic Packing Factor: FCC

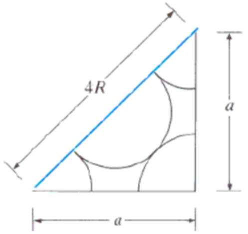
- APF for a face-centered cubic structure = 0.74

  maximum achievable APF



Close-packed directions:
length = $4R = \sqrt{2}\,a$

Unit cell contains:
$6 \times 1/2 + 8 \times 1/8$
= 4 atoms/unit cell

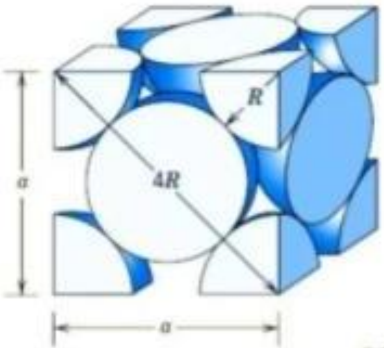


$$\text{APF} = \frac{\overbrace{4}^{\text{atoms/unit cell}}\ \overbrace{\frac{4}{3}\pi(\sqrt{2}a/4)^3}^{\text{volume/atom}}}{\underbrace{a^3}_{\text{volume/unit cell}}}$$

Face – Centred cubic unit cell (FCC)

Determination of FCC Unit Cell Volume

Calculate the volume of an FCC unit cell in terms of the atomic radius R.



- the atoms touch one another across a face-diagonal the length of which is $4R$.
- Since the unit cell is a cube, its volume is a^3 Where 'a' cell edge length.
- From the right triangle on the face,

$$a^2 + a^2 = (4R)^2$$

or, solving for a,

$$a = 2R\sqrt{2}$$

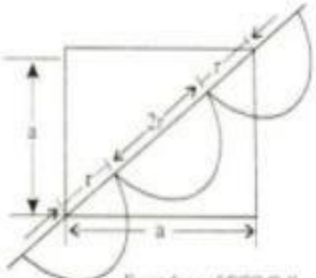
The FCC unit cell volume V_C may be computed from

$$V_C = a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2}$$

Atomic Packing Factor for FCC

Solution

$$\text{APF} = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}} = \frac{V_S}{V_C}$$



Front face of FCC Cell

The total atom and unit cell volumes may be calculated in terms of the atomic radius R.

The volume for a sphere is - $\frac{4}{3}\pi R^3$

since there are 4 atoms per FCC unit cell, the total FCC atom (or sphere) volume is,

$$V_S = (4)\tfrac{4}{3}\pi R^3 = \tfrac{16}{3}\pi R^3$$

total unit cell volume is $V_C = 16R^3\sqrt{2}$

Therefore, the atomic packing factor is $\text{APF} = \frac{V_S}{V_C} = \frac{\left(\frac{16}{3}\right)\pi R^3}{16R^3\sqrt{2}} = 0.74$

Density of unit cell

$$\text{Density of the unit cell } \rho = \frac{\text{mass of the unit cell}}{\text{volume of the unit cell}} \quad ...(1)$$

$$\text{mass of the unit cell} = \left\{\begin{array}{l}\text{total number of} \\ \text{atoms belongs to} \\ \text{that unit cell}\end{array}\right\} \times \left\{\begin{array}{l}\text{mass of} \\ \text{one atom}\end{array}\right\} \quad ...(2)$$

$$\text{mass of one atom} = \frac{\text{molar mass (gmol}^{-1}\text{)}}{\text{Avagadro number (mol}^{-1}\text{)}}$$

$$m = \frac{M}{N_A} \quad ...(3)$$

Substitute (3) in (2)

$$\text{mass of the unit cell} = n \times \frac{M}{N_A} \quad ...(4)$$

For a cubic unit cell, all the edge lengths are equal i.e , a=b=c

$$\text{volume of the unit cell} = a \times a \times a = a^3 \quad ...(5)$$

$$\therefore \textbf{ Density of the unit cell } \rho = \frac{n\,M}{a^3 N_A} \quad ...(6)$$

Problem #4

THE COPPER (FCC) CRYSTAL Consider the FCC unit cell of the copper crystal shown in Figure

a. How many atoms are there per unit cell?

b. If R is the radius of the Cu atom, show that the lattice parameter a is given by $a = R2\sqrt{2}$.

c. Calculate the **atomic packing factor** (APF) defined by

$$\text{APF} = \frac{\text{Volume of atoms in unit cell}}{\text{Volume of unit cell}}$$

d. Calculate the **atomic concentration** (number of atoms per unit volume) in Cu and the density of the crystal given that the atomic mass of Cu is 63.55 g mol^{-1} and the radius of the Cu atom is 0.128 nm.

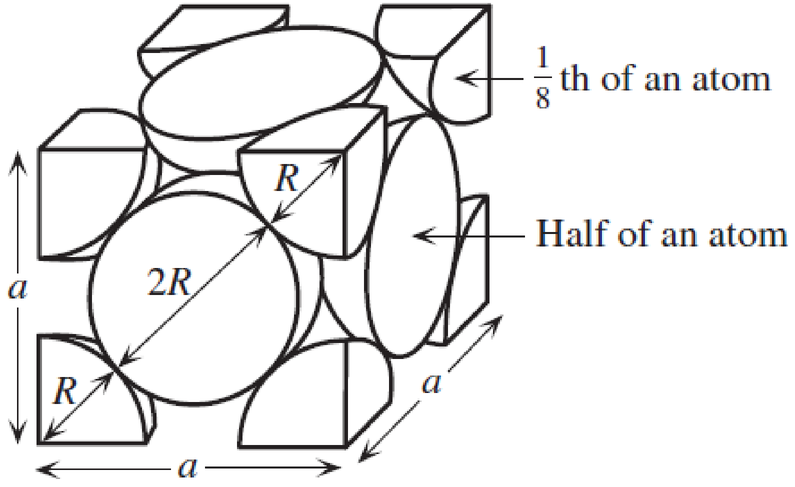


Figure The FCC unit cell.
The atomic radius is R and the lattice parameter is a.

SOLUTION

a. There are four atoms per unit cell. The Cu atom at each corner is shared with eight other adjoining unit cells. Each Cu atom at the face center is shared with the neighboring unit cell. Thus, the number of atoms in the unit cell = 8 corners ($\frac{1}{8}$ atom) + 6 faces ($\frac{1}{2}$ atom) = 4 atoms.

b. Consider the unit cell shown in Figure and one of the cubic faces. The face is a square of side a and the diagonal is $\sqrt{a^2 + a^2}$ or $a\sqrt{2}$. The diagonal has one atom at the center of diameter $2R$, which touches two atoms centered at the corners. The diagonal, going from corner to corner, is therefore $R + 2R + R$. Thus, $4R = a\sqrt{2}$ and $a = 4R/\sqrt{2} = R2\sqrt{2}$. Therefore, $a = 0.3620$ nm.

c.

$$\text{APF} = \frac{(\text{Number of atoms in unit cell}) \times (\text{Volume of atom})}{\text{Volume of unit cell}}$$

$$= \frac{4 \times \frac{4}{3}\pi R^3}{a^3} = \frac{\frac{4^2}{3}\pi R^3}{(R2\sqrt{2})^3} = \frac{4^2\pi}{3(2\sqrt{2})^3} = 0.74$$

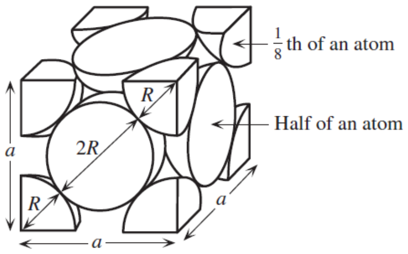


Figure The FCC unit cell. The atomic radius is R and the lattice parameter is a.

d. In general, if there are x atoms in the unit cell, the atomic concentration is

$$n_{at} = \frac{\text{Number of atoms in unit cell}}{\text{Volume of unit cell}} = \frac{x}{a^3}$$

Thus, for Cu

$$n_{at} = \frac{4}{(0.3620 \times 10^{-7}\ \text{cm})^3} = 8.43 \times 10^{22}\ \text{cm}^{-3}$$

There are x atoms in the unit cell, and each atom has a mass of M_{at}/N_A grams. The density ρ is

$$\rho = \frac{\text{Mass of all atoms in unit cell}}{\text{Volume of unit cell}} = \frac{x\left(\dfrac{M_{at}}{N_A}\right)}{a^3}$$

that is,

$$\rho = \frac{n_{at}M_{at}}{N_A} = \frac{(8.43 \times 10^{22}\ \text{cm}^{-3})(63.55\ \text{g mol}^{-1})}{6.022 \times 10^{23}\ \text{mol}^{-1}} = 8.9\ \text{g cm}^{-3}$$

Problem #5

Calculate the drift mobility and the mean scattering time of conduction electrons in copper at room temperature, given that the conductivity of copper is $5.9 \times 10^5\ \Omega^{-1}\ \text{cm}^{-1}$. [$n = 8.5 \times 10^{22}$ electrons cm^{-3}.]

Solution :

The electron drift mobility is

$$\mu_d = \frac{\sigma}{en} = \frac{5.9 \times 10^5\ \Omega^{-1}\ \text{cm}^{-1}}{[(1.6 \times 10^{-19}\ \text{C})(8.5 \times 10^{22}\ \text{cm}^{-3})]}$$

$$= 43.4\ \text{cm}^2\ \text{V}^{-1}\ \text{s}^{-1}$$

From the drift mobility we can calculate the mean free time τ between collisions by using Equation

$$\tau = \frac{\mu_d m_e}{e} = \frac{(43.4 \times 10^{-4}\ \text{m}^2\ \text{V}^{-1}\ \text{s}^{-1})(9.1 \times 10^{-31}\ \text{kg})}{1.6 \times 10^{-19}\ \text{C}} = 2.5 \times 10^{-14}\ \text{s}$$

Problem #6

What is the applied electric field that will impose a drift velocity equal to 0.1 percent of the mean speed '$\boldsymbol{u}$'($\sim 10^6$ m s^{-1})of conduction electrons in copper? What is the corresponding current density and current through a Cu wire of diameter 1 mm? [μ_d is the drift mobility, which for copper is 43.4 cm^2 V^{-1} s^{-1} and $\sigma = 5.9 \times 10^7\ \Omega^{-1}$ m^{-1}]

Solution :

The drift velocity of the conduction electrons is

$$V_{dx} = \mu_d E_x$$

where μ_d is the drift mobility, which for copper is 43.4 cm2 V^{-1} s^{-1}

With $V_{dx} = 0.001u = 10^3$ m s^{-1},

$$E_x = \frac{v_{dx}}{\mu_d} = \frac{10^3 \text{ m s}^{-1}}{43.4 \times 10^{-4} \text{ m}^2 \text{ V}^{-1} \text{ s}^{-1}} = 2.3 \times 10^5 \text{ V m}^{-1} \quad \text{or} \quad 2.3 \text{ kV cm}^{-1}$$

$$
\begin{aligned}
J_x &= \sigma \mathbf{E}_x \\
&= \left(5.9 \times 10^{7}\ \Omega^{-1} m^{-1}\right)\left(2.3 \times 105\ V\ m^{-1}\right) \\
&= 1.4 \times 10^{13}\ A\ m^{-2} \text{ or } 1.4 \times 10^{7}\ A\ mm^{-2}
\end{aligned}
$$

Problem #7

A brass disk of electrical resistivity 50 nΩ m conducts heat from a heat source to a heat sink at a rate of 10 W. If its diameter is 20 mm and its thickness is 30 mm, what is the temperature drop across the disk, neglecting the heat losses from the surface?

SOLUTION

We first determine the thermal conductivity:

$$\kappa = \sigma T C_{\mathrm{WFL}} = (5 \times 10^{-8}\ \Omega\ \mathrm{m})^{-1}(300\ \mathrm{K})(2.44 \times 10^{-8}\ \mathrm{W}\ \Omega\ \mathrm{K}^{-2})$$
$$= 146\ \mathrm{W\ m^{-1}\ K^{-1}}$$

The thermal resistance is

$$\theta = \frac{L}{\kappa A} = \frac{(30 \times 10^{-3}\ \mathrm{m})}{(146\ \mathrm{W\ m^{-1}\ K^{-1}})\pi(10 \times 10^{-3}\ \mathrm{m})^2} = 0.65\ \mathrm{K\ W^{-1}}$$

Therefore, the temperature drop is

$$\Delta T = \theta Q' = (0.65\ \mathrm{K\ W^{-1}})(10\ \mathrm{W}) = 6.5\ \mathrm{K\ or\ ^\circ C}$$