

$$= 5.72 \times 10^{22} \text{ atoms/cm}^3$$

Now, from Equation 4.1, the total number of vacancies, N_v , is computed as

$$\begin{aligned} N_v &= N_{\text{Au}} \exp\left(-\frac{Q_v}{kT}\right) \\ &= (5.72 \times 10^{22} \text{ atoms/cm}^3) \exp\left[-\frac{0.98 \text{ eV/atom}}{(8.62 \times 10^{-5} \text{ eV/K})(800 + 273 \text{ K})}\right] \\ &= 1.432 \times 10^{18} \text{ vacancies/cm}^3 \end{aligned}$$

We now want to determine the number of vacancies per unit cell, which is possible if the unit cell volume is multiplied by N_v . The unit cell volume (V_C) may be calculated using Equation 3.5 taking $n = 4$ inasmuch as Au has the FCC crystal structure. Thus, from a rearranged form of Equation 3.5

$$\begin{aligned} V_C &= \frac{nA_{\text{Au}}}{\rho_{\text{Au}} N_A} \\ &= \frac{(4 \text{ atoms/unit cell})(196.97 \text{ g/mol})}{(18.699 \text{ g/cm}^3)(6.023 \times 10^{23} \text{ atoms/mol})} \\ &= 6.996 \times 10^{-23} \text{ cm}^3/\text{unit cell} \end{aligned}$$

Now, the number of vacancies per unit cell, n_v , is just

$$\begin{aligned} n_v &= N_v V_C \\ &= (1.432 \times 10^{18} \text{ vacancies/cm}^3)(6.996 \times 10^{-23} \text{ cm}^3/\text{unit cell}) \\ &= 0.0001002 \text{ vacancies/unit cell} \end{aligned}$$

What this means is that instead of there being 4.0000 atoms per unit cell, there are only $4.0000 - 0.0001002 = 3.9998998$ atoms per unit cell. And, finally, the density may be computed using Equation 3.5 taking $n = 3.9998998$; thus