Solution to Exercise 3.1-1: "Calculate Geometry Factors"

The geometry factor (always for a single vacancy) was defined as

$$g = \frac{1}{2} \cdot \sum_{i} \left(\frac{\Delta x_{i}}{a} \right)^{2}$$

- With Δx_i = component of the jump in x-direction.
- Looking at the fcc lattice we realize that there are 12 possibilities for a jump because there are 12 next neighbors.
 - **8** of the possible jumps have a component in x (or -x) -direction, and $\Delta x_i = a/2$
 - We thus have

$$g_{fcc} = \frac{1}{2} \cdot 8 \cdot \left(\frac{1}{2}\right)^2 = 1$$

- Looking at the bcc lattice we realize that there are 8 possibilities for a jump because there are 8 next neighbors.
 - All 8 possible jumps have the component $\Delta x_i = a/2$ in x-direction, again we have

$$g_{bcc} = \frac{1}{2} \cdot 8 \cdot \left(\frac{1}{2}\right)^2 = 1$$

- Looking at the <u>diamond lattice</u> we realize, after a bit more thinking (or drawing, or looking at a ball and stick model), that there are **4** possible jumps.
 - All 4 jumps have the component $\Delta x_i = a/4$ in x-direction, and we obtain

$$g_{\text{ diamond}} = \frac{1}{2} \cdot 4 \cdot \left(\frac{1}{4}\right)^2 = \frac{1}{8}$$