PHYS4061 Computational Physics 2024-2025
Homework 01

Name: WAN Chi Kit
SID: 1155158885

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Problem 1.1

By the definition of reciprocal lattices:

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$
\begin{aligned}
\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) &= 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \cdot (\vec{b}_2 \times \vec{b}_3) \\
&= 2\pi \frac{(\vec{a}_2 \times \vec{a}_3) \cdot (\vec{b}_2 \times \vec{b}_3)}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \\
&= 2\pi \frac{(\vec{a}_2 \cdot \vec{b}_2)(\vec{a}_3 \cdot \vec{b}_3) - (\vec{a}_2 \cdot \vec{b}_3)(\vec{a}_3 \cdot \vec{b}_2)}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \\
&= 2\pi \frac{2\pi\delta_{22} \cdot 2\pi\delta_{33} - 2\pi\delta_{23} \cdot 2\pi\delta_{32}}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \\
&= 2\pi \frac{(2\pi)^2 - 0}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \\
&= \frac{(2\pi)^3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}
\end{aligned}
$$

Problem 1.2

$$
\begin{aligned}
2\pi\frac{\vec{b}_2\times\vec{b}_3}{\vec{b}_1\cdot(\vec{b}_2\times\vec{b}_3)} &= 2\pi\frac{\vec{b}_2}{\vec{b}_1\cdot(\vec{b}_2\times\vec{b}_3)}\times\vec{b}_3 \\
&= 2\pi\frac{\vec{b}_2}{\vec{b}_1\cdot(\vec{b}_2\times\vec{b}_3)}\times 2\pi\frac{\vec{a}_1\times\vec{a}_2}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)} \\
&= (2\pi)^2\frac{\vec{b}_2\times(\vec{a}_1\times\vec{a}_2)}{[\vec{b}_1\cdot(\vec{b}_2\times\vec{b}_3)][\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)]} \\
&= (2\pi)^2\frac{\vec{a}_1(\vec{b}_2\cdot\vec{a}_2)-\vec{a}_2(\vec{b}_2\times\vec{a}_1)}{[\vec{b}_1\cdot(\vec{b}_2\times\vec{b}_3)][\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)]} \\
&= (2\pi)^2\frac{2\pi\delta_{22}\vec{a}_1-2\pi\delta_{12}\vec{a}_2}{[\vec{b}_1\cdot(\vec{b}_2\times\vec{b}_3)][\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)]} \\
&= (2\pi)^3\frac{\vec{a}_1}{[\vec{b}_1\cdot(\vec{b}_2\times\vec{b}_3)][\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)]} \\
&= (2\pi)^3\frac{\vec{a}_1}{\frac{(2\pi)^3}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}[\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)]} \\
&= \vec{a}_1
\end{aligned}
$$

Problem 1.3

$$\text{packing fraction} = \frac{\text{total volume occupied by constituent particles}}{10^2\text{'s total volume}}$$

For BCC, the number of atoms per unit 10^2s is $\frac{1}{8} \times 8 + 1 = 2$, and the relation between edge length a and radius of atom r is $4r = \sqrt{2a^2 + a^2} \implies r = \frac{\sqrt{3}}{4}a$

$$\begin{aligned}
\text{packing fractionpacking fraction} = \frac{2 \times \frac{4}{3}\pi r^3}{a^3} &= \frac{2 \times \frac{4}{3}\pi\left(\frac{\sqrt{3}}{4}a\right)^3}{a^3} \\
&= \frac{2 \times \frac{4}{3}\pi \times \frac{3\sqrt{3}}{64}a^3}{a^3} \\
&= \frac{2 \times \frac{4}{3}\pi \times 3\sqrt{3}}{64} \\
&= \frac{8\sqrt{3}}{64}\pi \\
&= \frac{\sqrt{3}}{8}\pi
\end{aligned}$$

For FCC, the number of atoms per unit 10^2s is $\frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 4$, and the relation between edge length a and radius of atom r is $4r = \sqrt{a^2 + a^2} \implies r = \frac{\sqrt{2}}{4}a$

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

$$= \frac{4 \times \frac{4}{3}\pi \times \frac{2\sqrt{2}}{64}a^3}{a^3}$$

$$= \frac{4 \times \frac{4}{3}\pi \times 2\sqrt{2}}{64}$$

$$= \frac{32\sqrt{2}}{192}\pi$$

$$= \frac{\sqrt{2}}{6}\pi$$

For Diamond, the number of atoms per unit 10^2s is $\frac{1}{8} \times 8 + \frac{1}{2} \times 6 + 4 = 8$, and the relation between edge length a and radius of atom r is $r = \frac{\sqrt{3}}{8}a$

$$\text{packing fraction} = \frac{8 \times \frac{4}{3}\pi r^3}{a^3} = \frac{8 \times \frac{4}{3}\pi \left(\frac{\sqrt{3}}{8}a\right)^3}{a^3}$$

$$= \frac{8 \times \frac{4}{3}\pi \times \frac{3\sqrt{3}}{512}a^3}{a^3}$$

$$= \frac{8 \times \frac{4}{3}\pi \times 3\sqrt{3}}{512}$$

$$= \frac{32\sqrt{3}}{512}\pi$$

$$= \frac{\sqrt{3}}{16}\pi$$

Problem 1.4

Integrating $f(x) = x^8$ from $[-1, 1]$ using trapezoidal rule and random sampling,

$$I_{\text{exact}} = \int_{-1}^{1} x^8 dx = \frac{1}{9}x^9\Big|_{-1}^{1} = \frac{2}{9}$$

with

$$\text{squared deviation } sd = (I - I_{\text{exact}})^2$$

Here is the table of results,

N	sd of trapezoidal rule	sd of random sampling
10^2	2.84285e-07	0.00244528
10^3	2.84443e-11	0.000117882
10^4	2.84444e-15	6.41928e-06
10^5	2.84442e-19	2.17923e-07
10^6	2.81558e-23	5.13458e-10
10^7	4.50487e-26	2.76908e-09
10^8	1.07239e-23	4.89311e-10

By observation,

- The trapezoidal rule showed a lower squared deviation sd than random sampling consistently as N increases, meaning a higher accuracy
- A larger N does not always represent a lower squared deviation sd for both algorithm

For more details, please check the code attached.