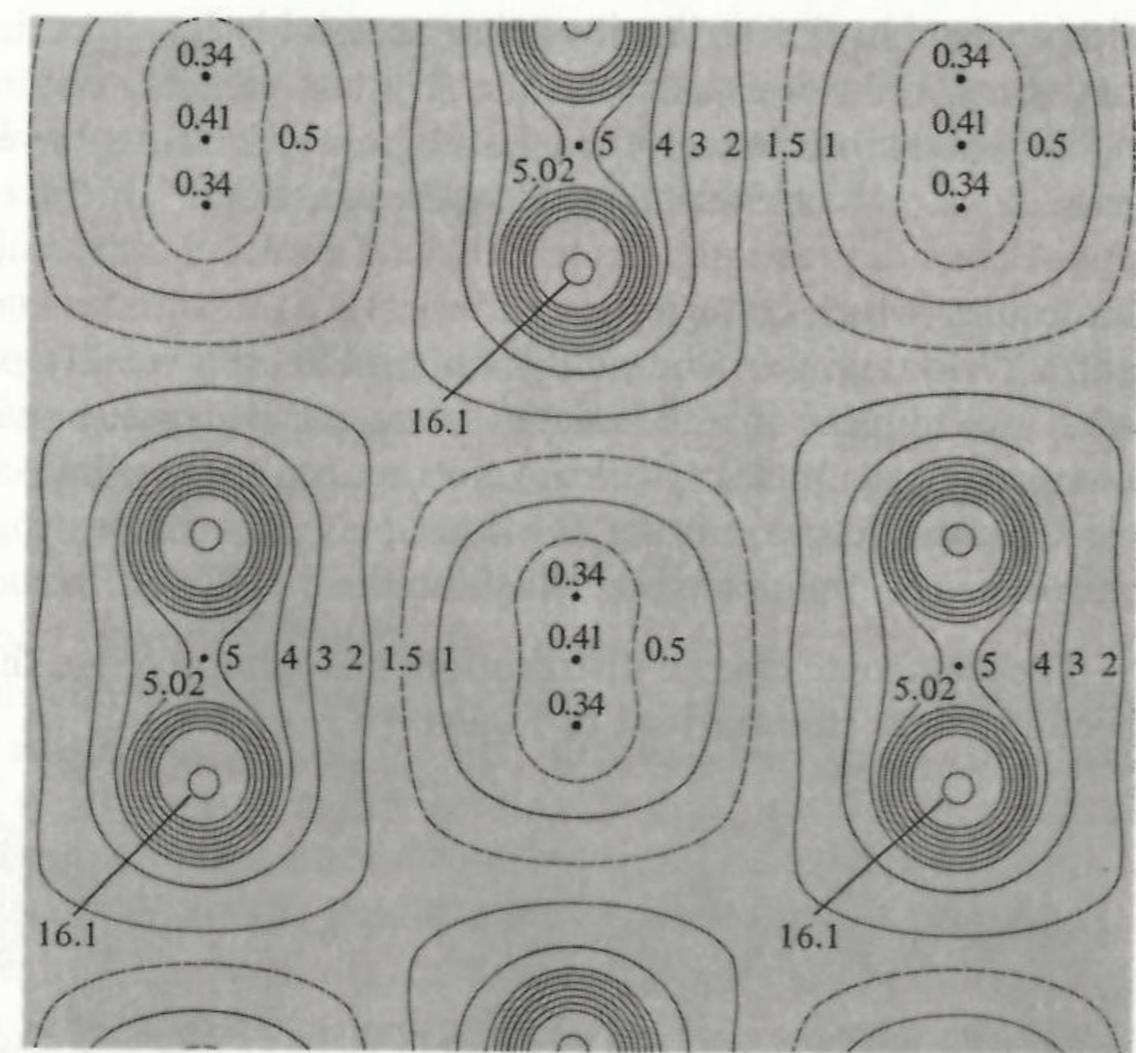
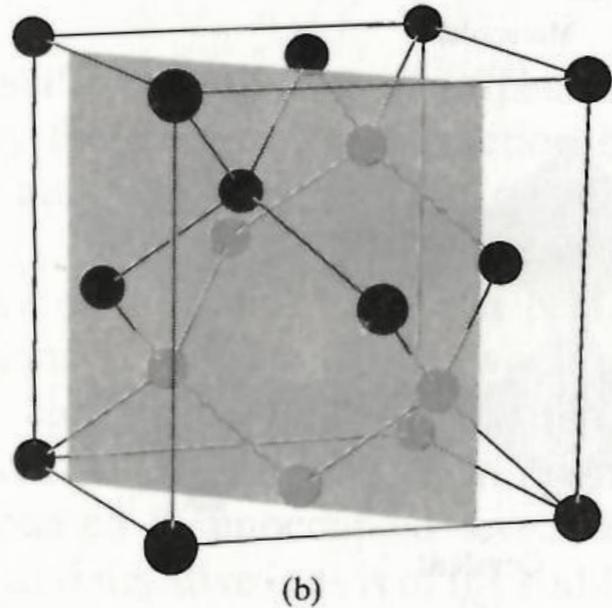


a)



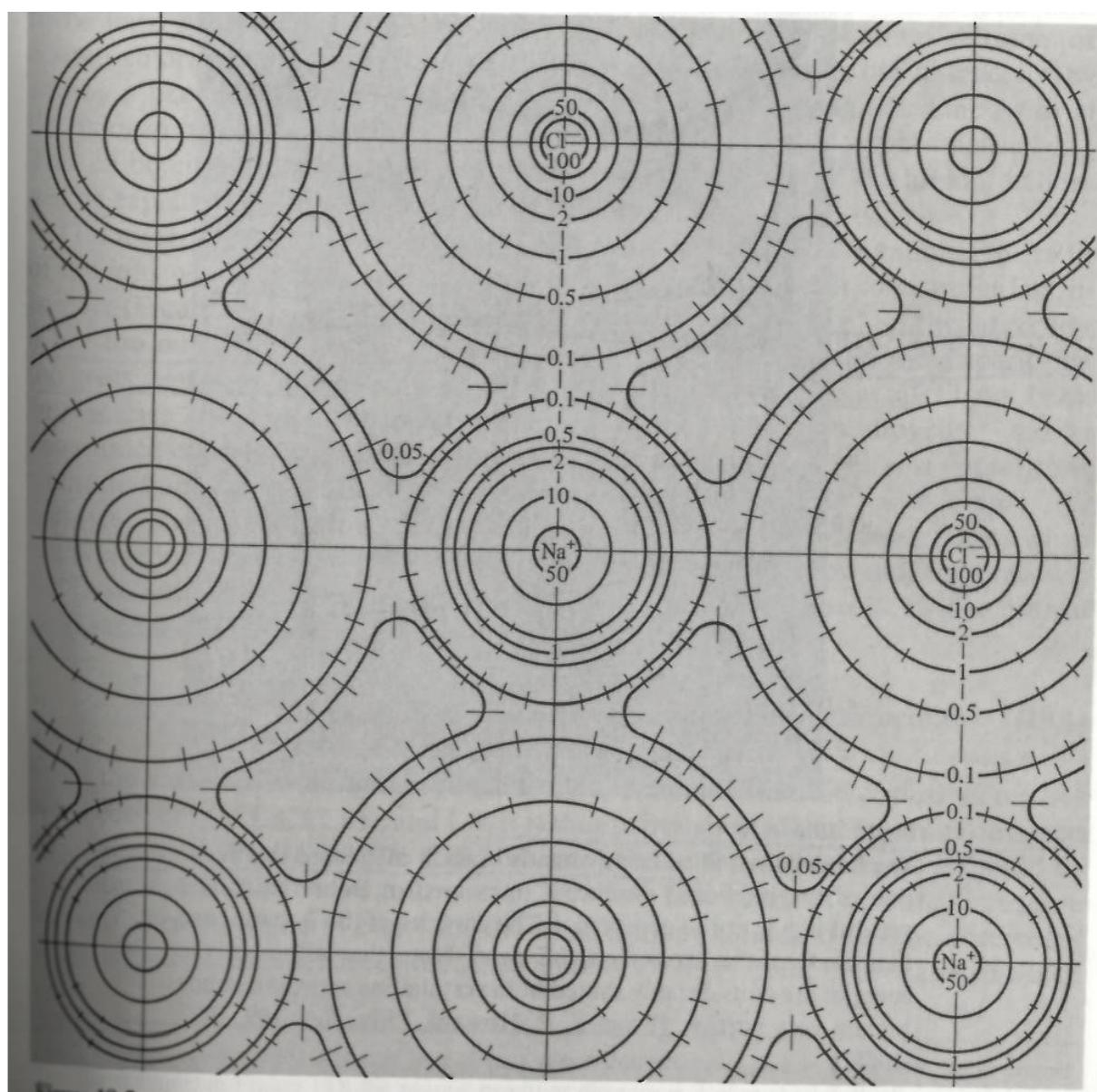
(a)



(b)

Which charge density represents
Covalent bonding?

b)



Question #1

What is the condition for constructive interference?

a) $2d \cos \theta = n\lambda$

b) $2d \sin \theta = n\lambda$

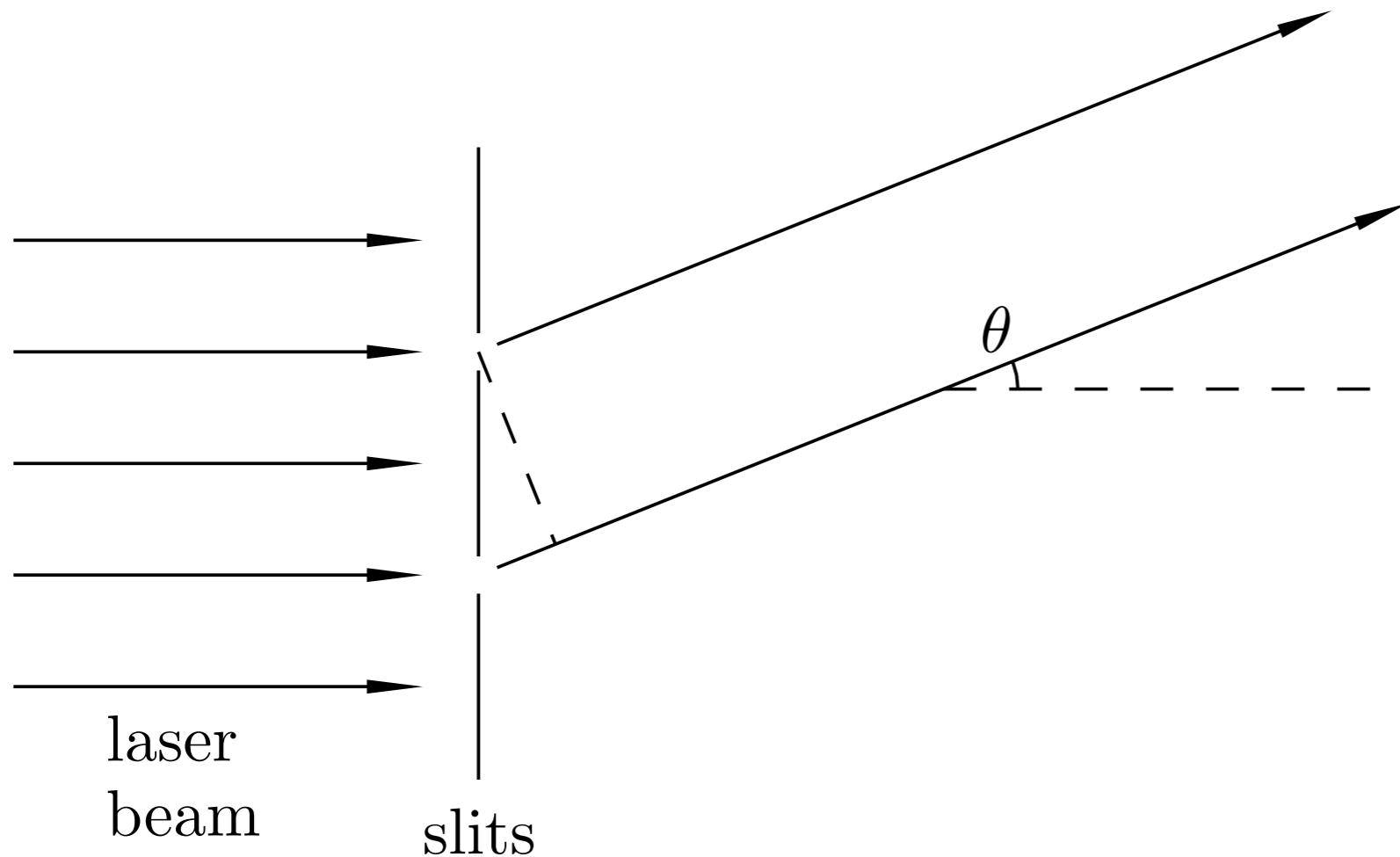
c) $\frac{d}{2} \sin \theta = n\lambda$

d) $d \cos \theta = n\lambda$

e) $d \sin \theta = n\lambda$

Question #1

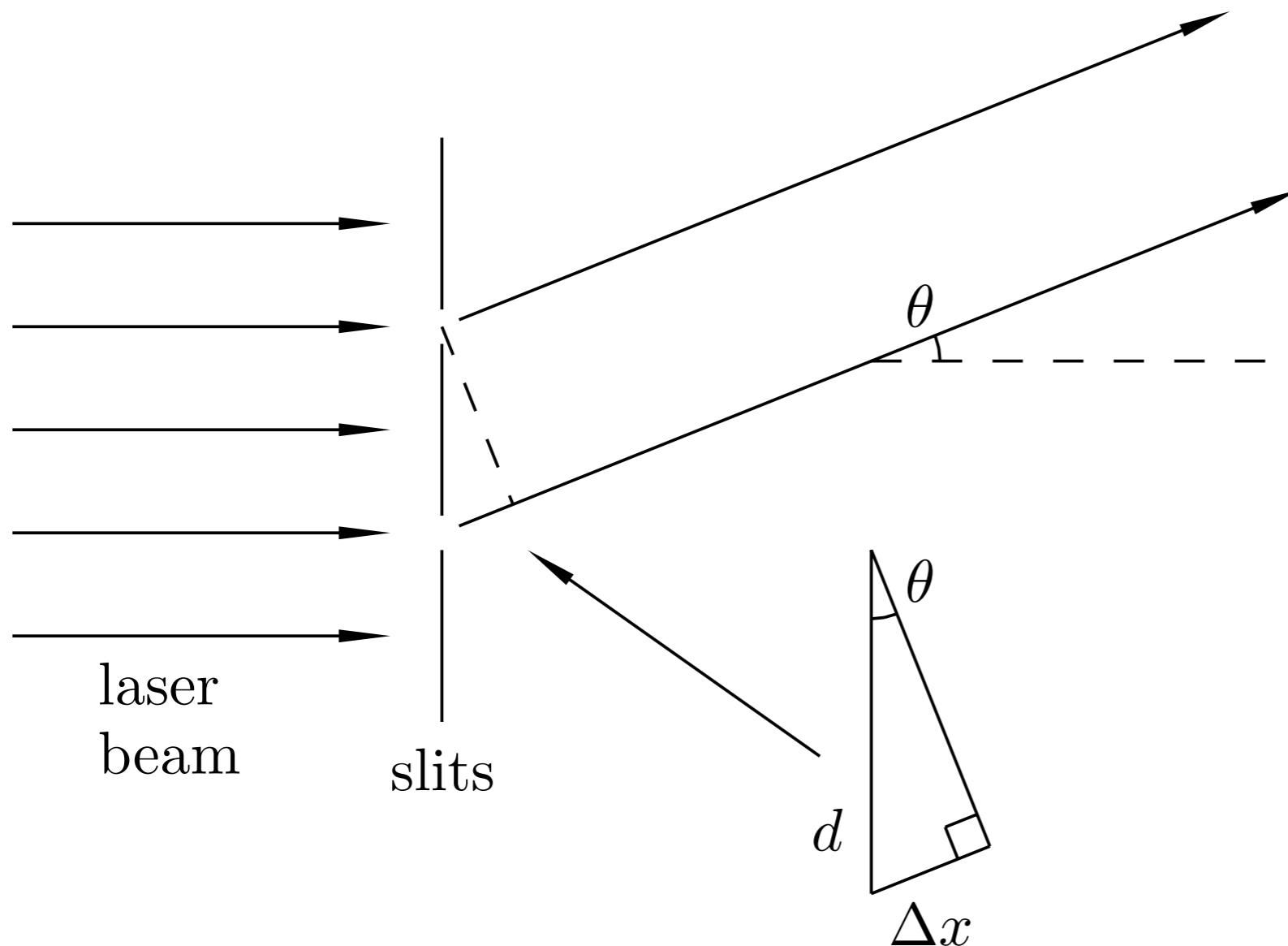
What is the condition for constructive interference?



- a) $2d \cos \theta = n\lambda$
- b) $2d \sin \theta = n\lambda$
- c) $\frac{d}{2} \sin \theta = n\lambda$
- d) $d \cos \theta = n\lambda$
- e) $d \sin \theta = n\lambda$

Question #1

What is the condition for constructive interference?



- a) $2d \cos \theta = n\lambda$
- b) $2d \sin \theta = n\lambda$
- c) $\frac{d}{2} \sin \theta = n\lambda$
- d) $d \cos \theta = n\lambda$
- e) $d \sin \theta = n\lambda$

Question #2

What is the value of “n” for
this peak?

$$d \sin \theta = n\lambda$$

- A. 1
- B. 2
- C. 4
- D. 6
- E. 5



Question #2

What is the value of “n” for
this peak?

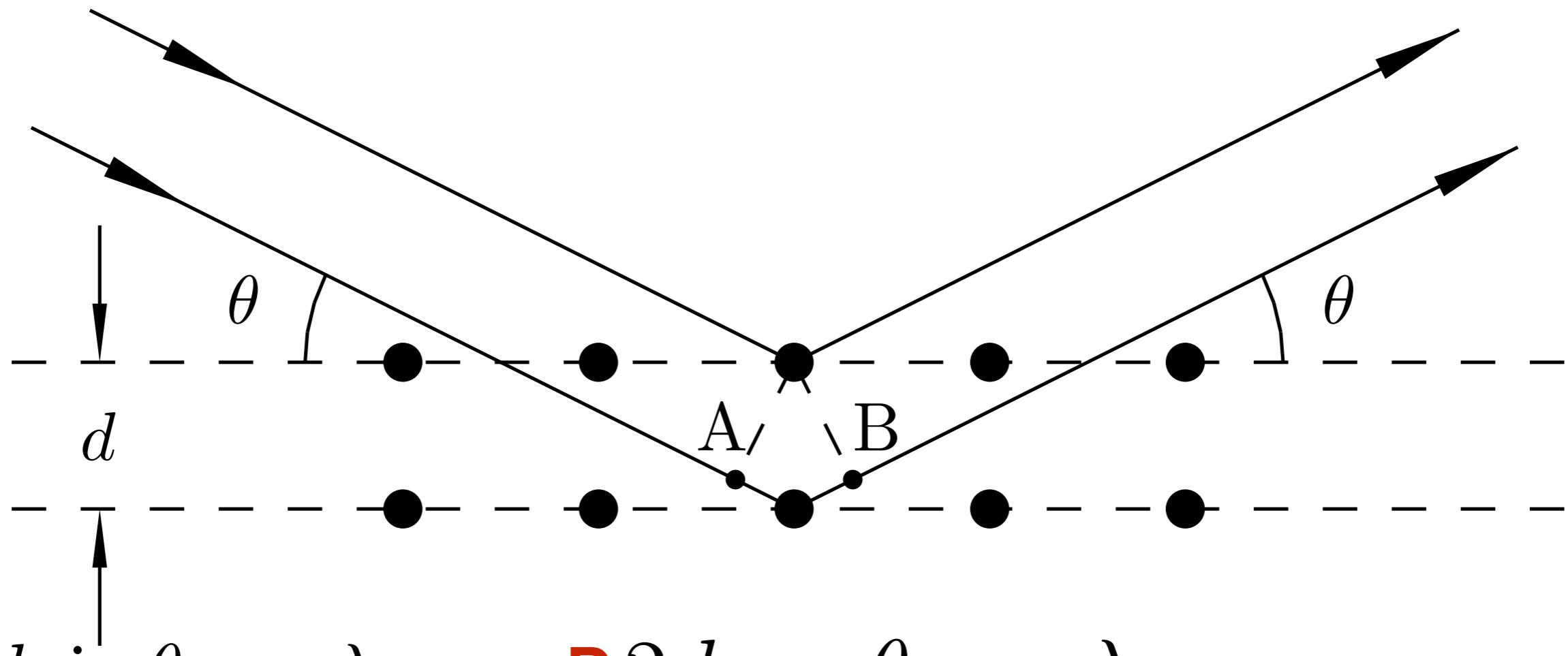
$$d \sin \theta = n\lambda$$

- A. 1
- B. 2
- C. 4
- D. 6
- E. 5



Question #3

What is the condition for constructive interference between these two light rays?



A $d \sin \theta = n\lambda$

B $\frac{d}{2} \sin \theta = n\lambda$

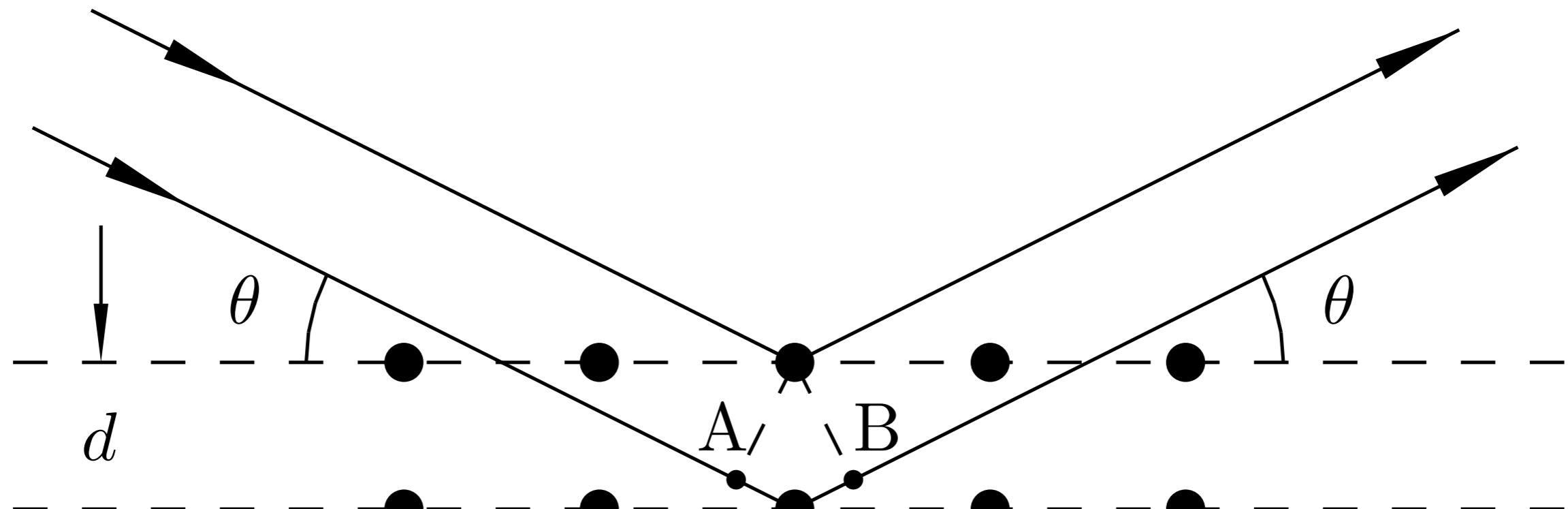
C $2d \sin \theta = n\lambda$

D $2d \cos \theta = n\lambda$

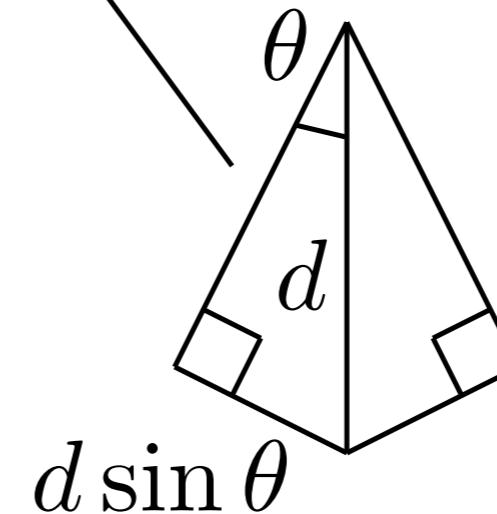
E $d \cos \theta = n\lambda$

Question #3

What is the condition for constructive interference between these two light rays?

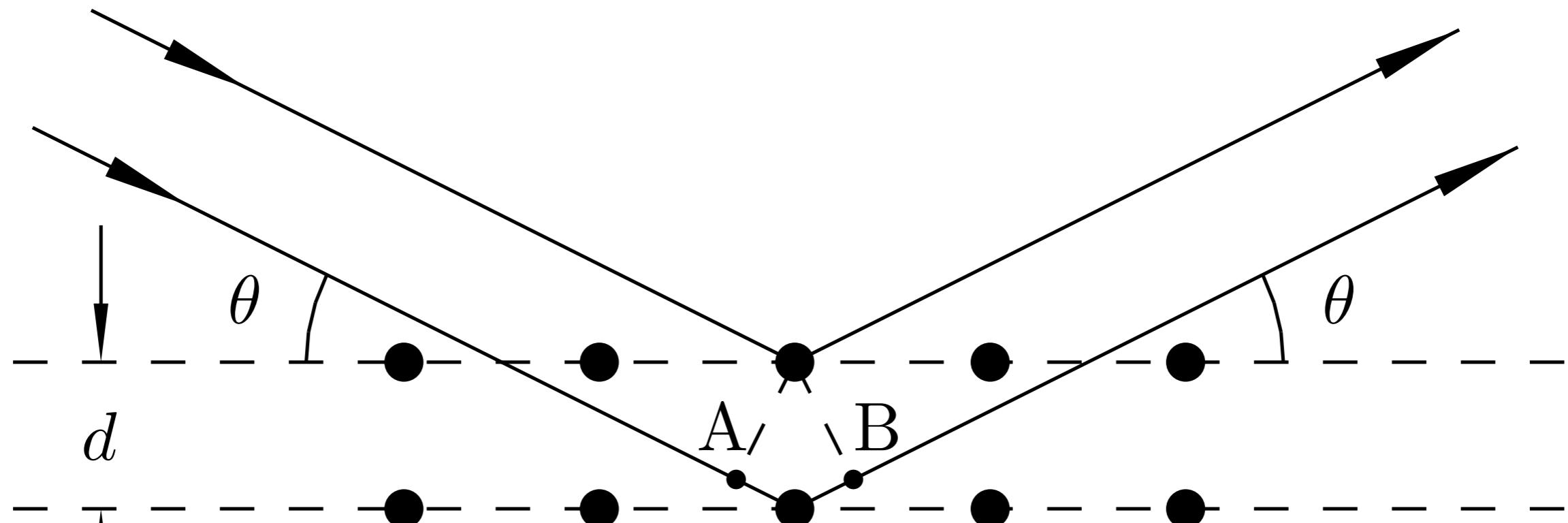


- A $d \sin \theta = n\lambda$
- B $\frac{d}{2} \sin \theta = n\lambda$
- C $2d \sin \theta = n\lambda$



Question #3

What is the condition for constructive interference between these two light rays?

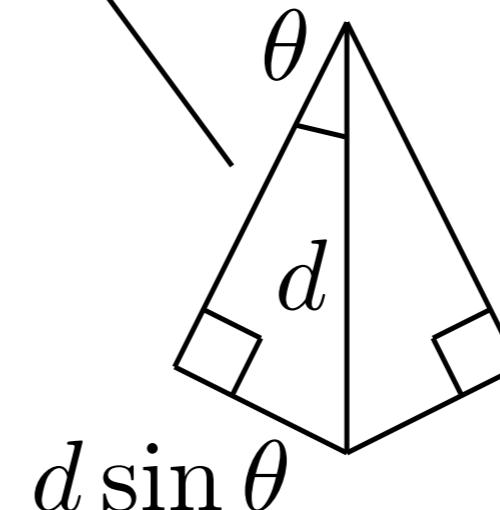


Bragg's Law

A $d \sin \theta = n\lambda$

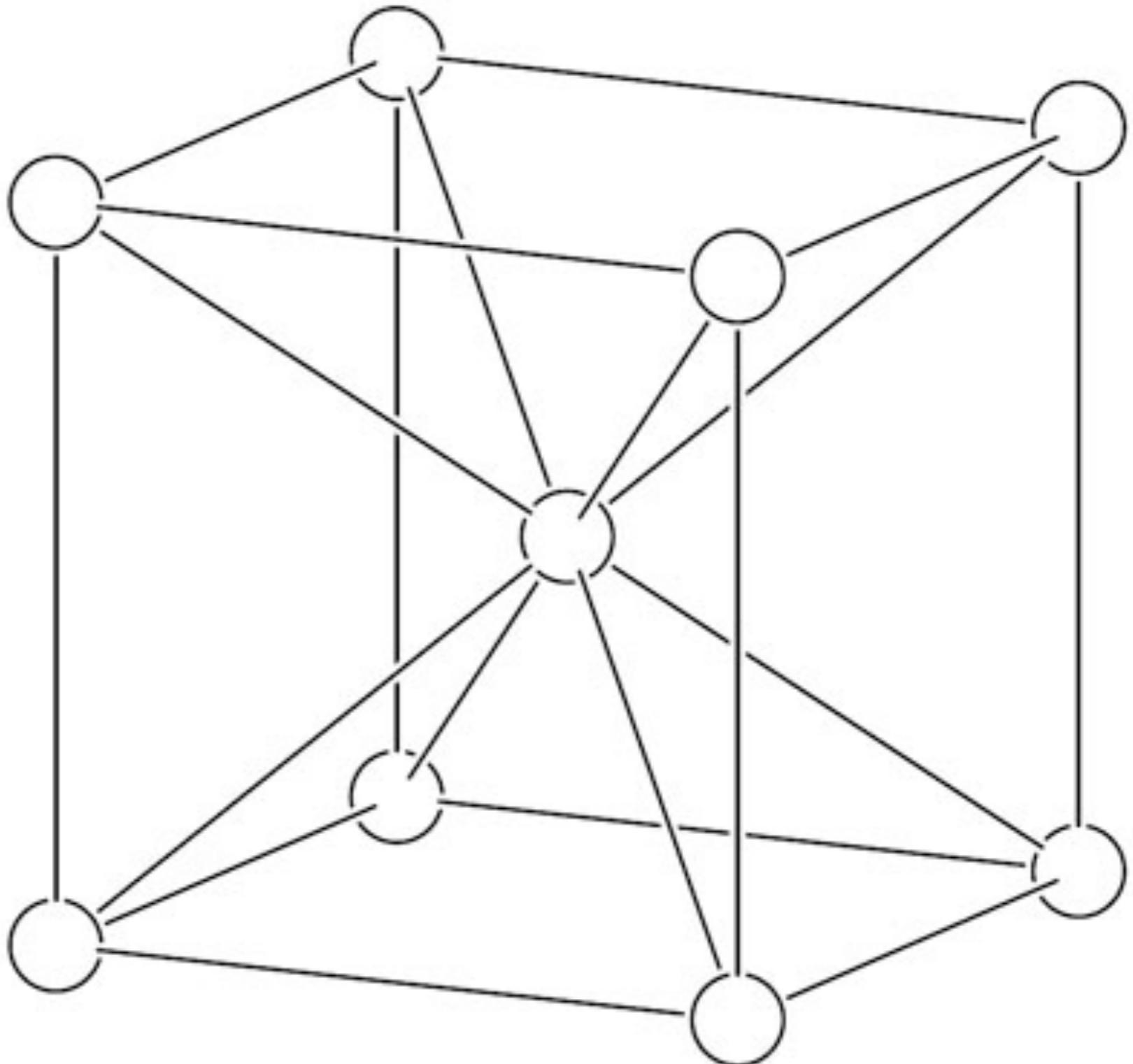
B $\frac{d}{2} \sin \theta = n\lambda$

C $2d \sin \theta = n\lambda$



Consider a bcc crystal with a lattice constant of 4.00 Å. Looking at the picture below, what is the spacing between (001) planes?

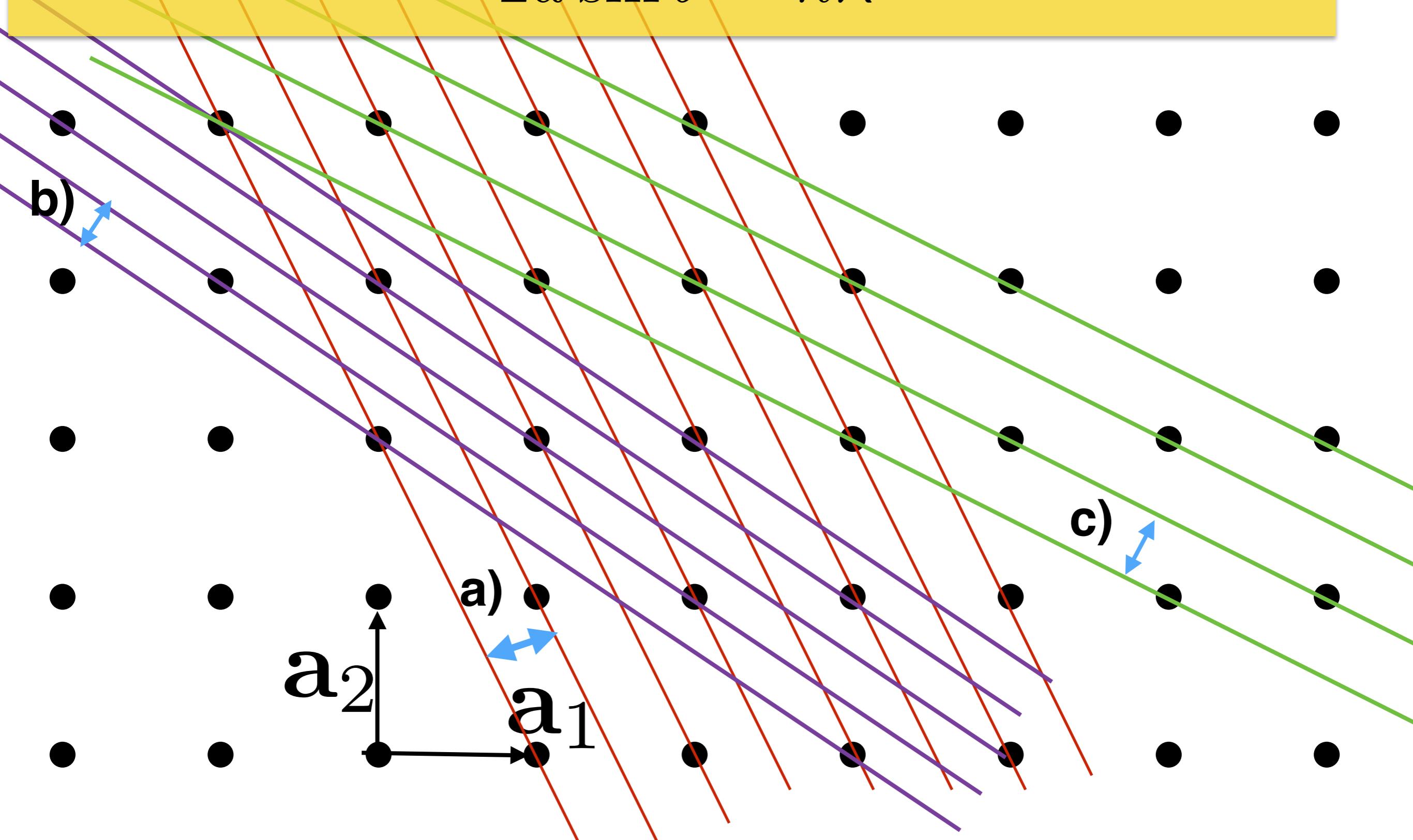
- A. 4.00 Å
- B. $\text{Sqrt}(3) \times 3.00$ Å
- C. $\text{Sqrt}(3) \times 4.00$ Å
- D. 2.00 Å
- E. $\text{Sqrt}(3) \times 2.00$ Å



Question #5

Which "d" should be used if you want to investigate diffraction from (210) planes?

$$2d \sin \theta = n\lambda$$



Let $d = 2.5$ Angstroms. At what angles do you observe Bragg peaks? How many angles did you

find (X-ray wavelength is 1.542 \AA)

$$2d \sin \theta = n\lambda$$

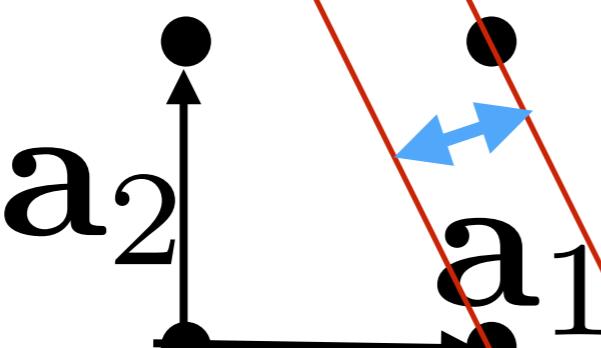
A. 1

B. 3

C. 4

D. 2

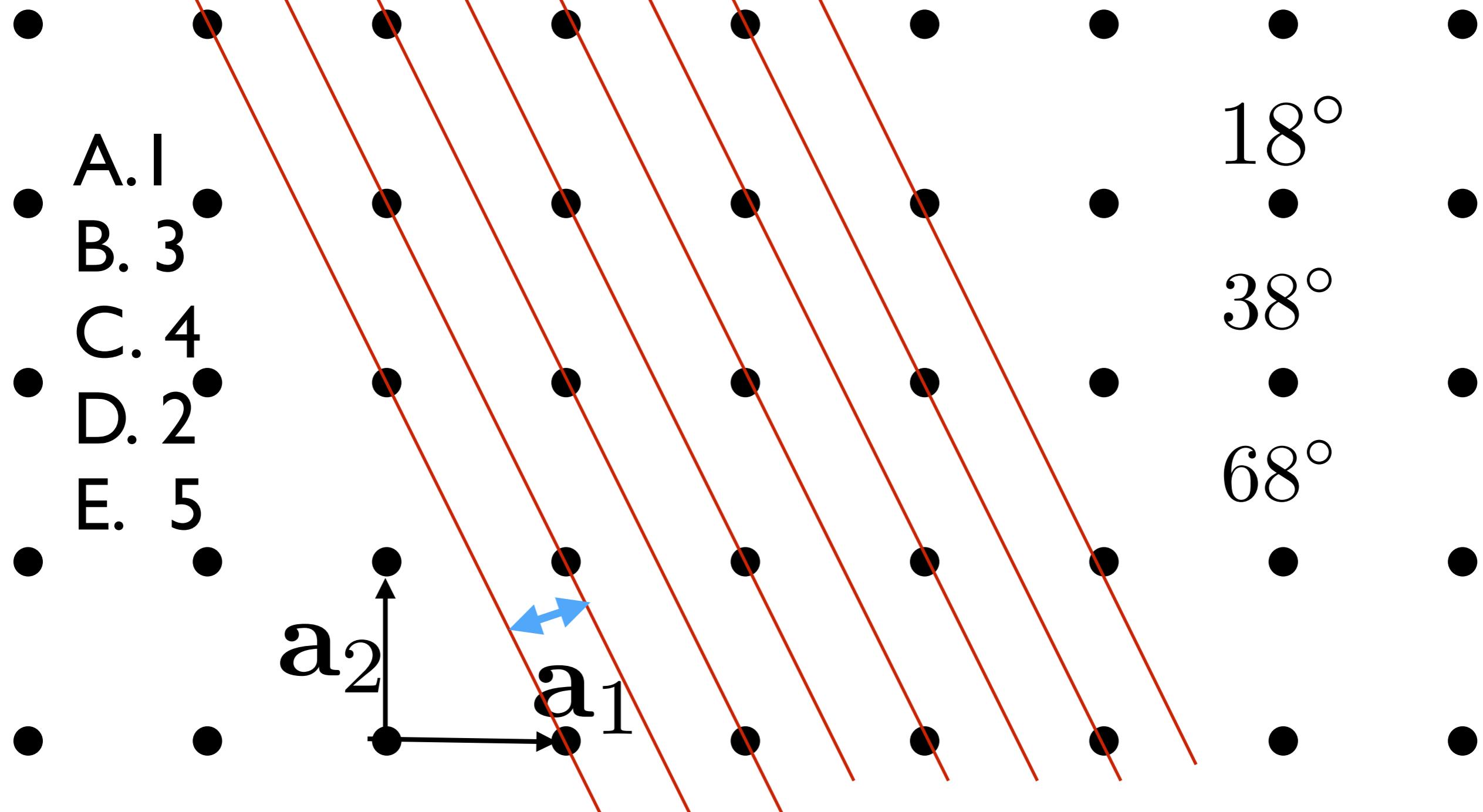
E. 5



Let $d = 2.5$ Angstroms. At what angles do you observe Bragg peaks? How many angles did you find?

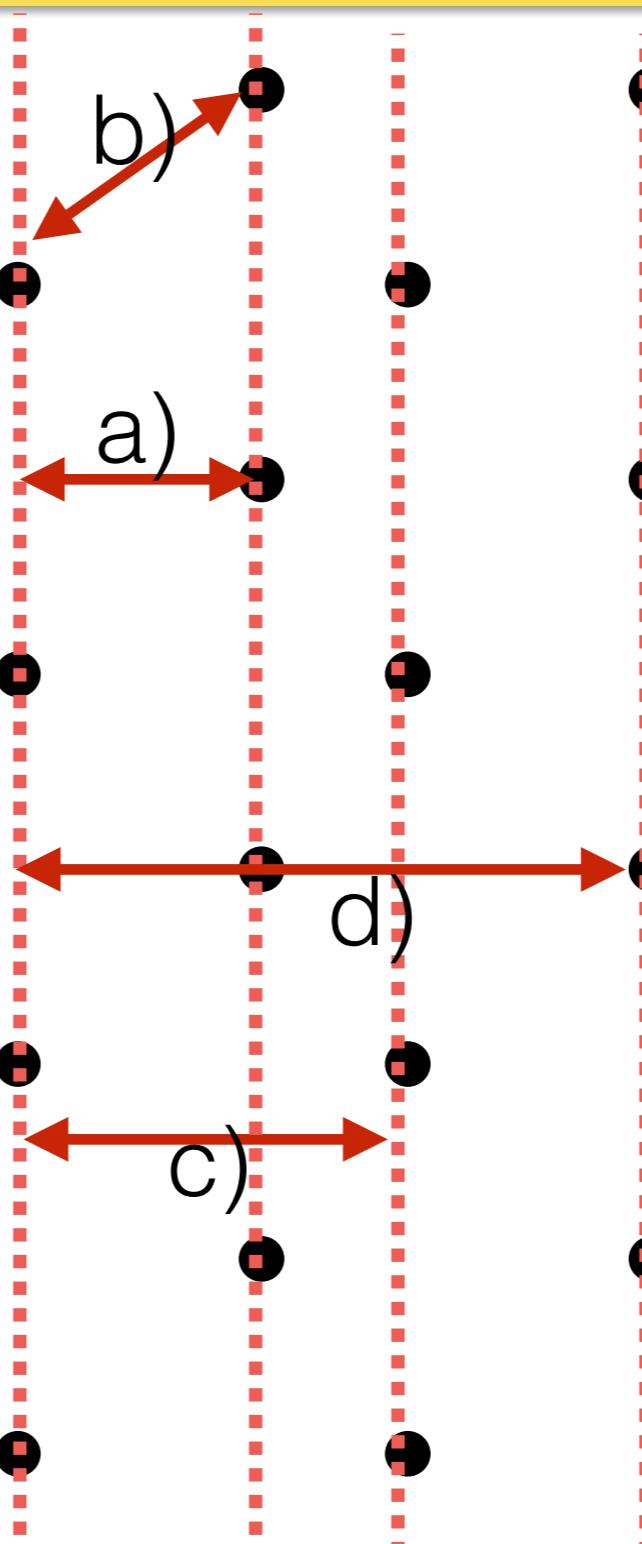
(X-ray wavelength is 1.542 \AA)

$$2d \sin \theta = n\lambda$$



Which “d” should be used if you want to investigate diffraction from (100) planes?

$$2d \sin \theta = n\lambda$$



At what angles do you observe Bragg peaks

- from (110) planes of atoms? How many angles did you find

$$2d \sin \theta = n\lambda \quad \lambda = 1.542 \text{ \AA}$$

(X-ray wavelength is 1.542 \AA)

Question #8



A. 1

B. 3

C. 4

D. 5

E. 2



$$a = 3.61 \text{ \AA}$$



Consider a crystal with atoms at the lattice points of a simple cubic lattice. If the lattice constant is 3.50 Å, at what angles will we observe Bragg peaks, scattered from (00l) planes, in an X-ray experiment? (X-ray wavelength is 1.542 Å)

Question #9

How many angles did you find?

- A. 1
- B. 3
- C. 4
- D. 2
- E. 5

Consider a crystal with atoms at the lattice points of a **body-centered** cubic lattice. If the lattice constant is 3.50 Å, at what angles will we observe Bragg peaks, scattered from (00l) planes, in an X-ray experiment? (X-ray wavelength is 1.542 Å)

Question #10

How many angles did you find?

- A. 1
- B. 5
- C. 3
- D. 4
- E. 2

Consider a CsCl crystal with a lattice constant of 3.50 Å, at what angles will we observe Bragg peaks, scattered from (00l) planes, in an X-ray experiment? (X-ray wavelength is 1.542 Å)

Question #11

How many angles did you find?

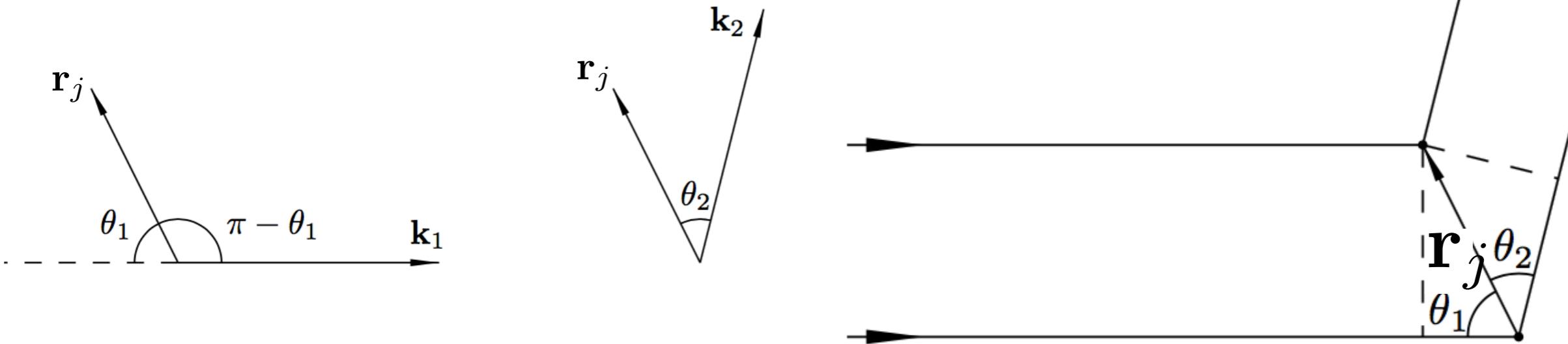
- A. 1
- B. 2
- C. 3
- D. 4
- E. 5

$$\mathcal{E}_1 \propto f_e(\theta) e^{ikr - i\omega t} \quad \boxed{1}$$

$$\mathcal{E}_2 \propto f_e(\theta) \frac{1}{r} e^{ikr - i\omega t + i\mathbf{r}_j \cdot \Delta \mathbf{k}} \quad \boxed{2}$$

$$\mathcal{E} \propto f_e(\theta) \frac{1}{r} e^{ikr - i\omega t} + f_e(\theta) \frac{1}{r} e^{ikr - i\omega t + i\mathbf{r}_j \cdot \Delta \mathbf{k}} \quad \boxed{3}$$

$$\mathcal{E} \propto f_e(\theta) [1 + e^{i\mathbf{r}_j \cdot \Delta \mathbf{k}}] \quad \boxed{4}$$



$$\boxed{5} \quad \mathcal{E} \propto f_e(\theta) \sum_j e^{i\mathbf{r}_j \cdot \Delta\mathbf{k}} \quad \boxed{6} \quad \mathcal{E} \propto f_e(\theta) \int \rho(\mathbf{r}) e^{i\mathbf{r} \cdot \Delta\mathbf{k}} d^3\mathbf{r}$$

$$\boxed{7} \quad \mathcal{E} \propto f_e(\theta) \sum_{\mathbf{R}} \sum_{\mathbf{r}_p} \int \rho(\mathbf{R} + \mathbf{r}_p + \mathbf{r}') e^{i(\mathbf{R} + \mathbf{r}_p + \mathbf{r}') \cdot \Delta\mathbf{k}} d^3\mathbf{r}'$$

$$\boxed{8} \quad \mathcal{E} \propto f_e(\theta) \sum_{\mathbf{R}} \sum_{\mathbf{r}_p} \int \rho(\mathbf{R} + \mathbf{r}_p + \mathbf{r}') e^{i\mathbf{R} \cdot \Delta\mathbf{k}} e^{i\mathbf{r}_p \cdot \Delta\mathbf{k}} e^{i\mathbf{r}' \cdot \Delta\mathbf{k}} d^3\mathbf{r}'$$

$$\boxed{9} \quad \mathcal{E} \propto f_e(\theta) \sum_{\mathbf{R}} \sum_{\mathbf{r}_p} \int \rho(\mathbf{r}_p + \mathbf{r}') e^{i\mathbf{R} \cdot \Delta\mathbf{k}} e^{i\mathbf{r}_p \cdot \Delta\mathbf{k}} e^{i\mathbf{r}' \cdot \Delta\mathbf{k}} d^3\mathbf{r}'$$

$$\boxed{10} \quad \mathcal{E} \propto f_e(\theta) \left[\sum_{\mathbf{R}} e^{i\mathbf{R} \cdot \Delta\mathbf{k}} \right] \sum_{\mathbf{r}_p} \int \rho(\mathbf{r}_p + \mathbf{r}') e^{i\mathbf{r}_p \cdot \Delta\mathbf{k}} e^{i\mathbf{r}' \cdot \Delta\mathbf{k}} d^3\mathbf{r}'$$

$$\boxed{11} \quad \mathcal{E} \propto f_e(\theta) \left[\sum_{\mathbf{R}} e^{i\mathbf{R} \cdot \Delta\mathbf{k}} \right] \sum_{\mathbf{r}_p} f_{ap}(\theta) e^{i\mathbf{r}_p \cdot \Delta\mathbf{k}}$$
$$f_{ap}(\theta) = \int \rho(\mathbf{r}_p + \mathbf{r}') e^{i\mathbf{r}' \cdot \Delta\mathbf{k}} d^3\mathbf{r}' \quad \boxed{12}$$

Big Deal!!

$$\mathcal{E} \propto f_e(\theta) \left[\sum_{\mathbf{R}} e^{i\mathbf{R} \cdot \Delta \mathbf{k}} \right] \sum_{\mathbf{r}_p} f_{ap}(\theta) e^{i\mathbf{r}_p \cdot \Delta \mathbf{k}}$$

$$\mathbf{G} = \Delta \mathbf{k}$$

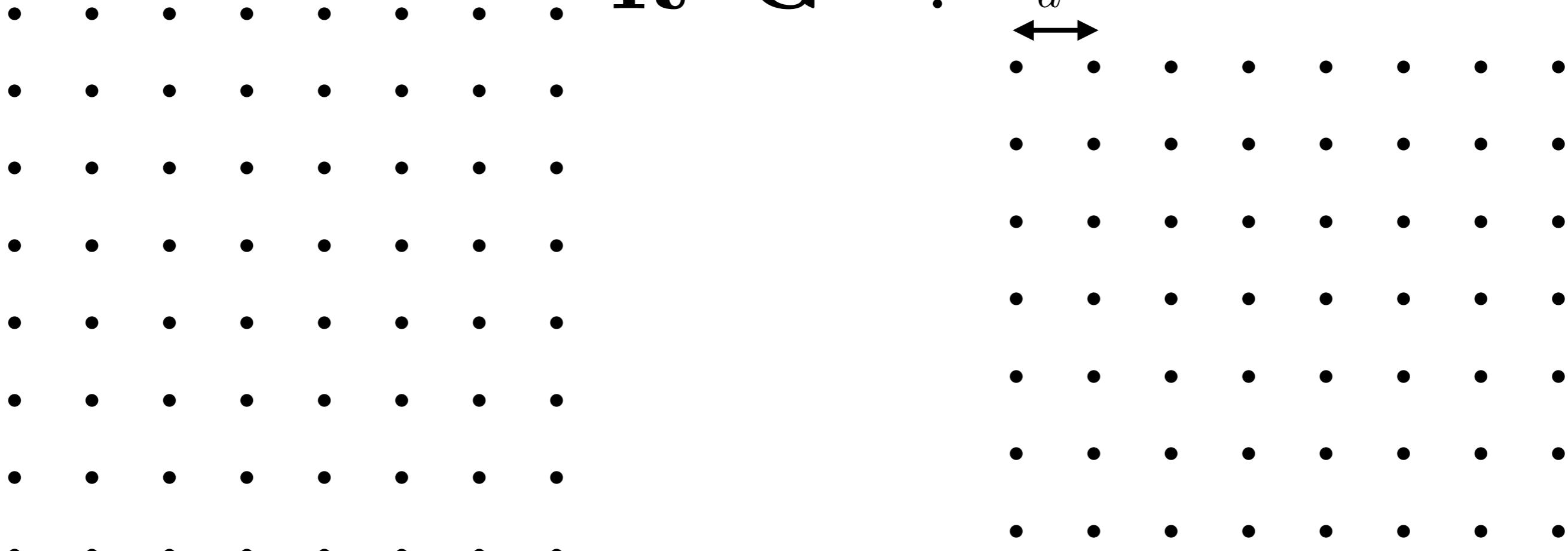
$$\mathbf{R} \cdot \mathbf{G} = ?$$

Big Deal!!

$$\mathcal{E} \propto f_e(\theta) \left[\sum_{\mathbf{R}} e^{i\mathbf{R} \cdot \Delta \mathbf{k}} \right] \sum_{\mathbf{r}_p} f_{ap}(\theta) e^{i\mathbf{r}_p \cdot \Delta \mathbf{k}}$$

$$\mathbf{G} = \Delta \mathbf{k}$$

$$\text{---} \xrightarrow{a} \text{---} \quad \mathbf{R} \cdot \mathbf{G} = ? \quad \frac{2\pi}{a} \text{---} \xrightarrow{2\pi/a} \text{---}$$



Big Deal!!

$$\mathcal{E} \propto f_e(\theta) \left[\sum_{\mathbf{R}} e^{i\mathbf{R} \cdot \Delta\mathbf{k}} \right] \sum_{\mathbf{r}_p} f_{ap}(\theta) e^{i\mathbf{r}_p \cdot \Delta\mathbf{k}}$$

$$\mathbf{G} = \Delta\mathbf{k}$$

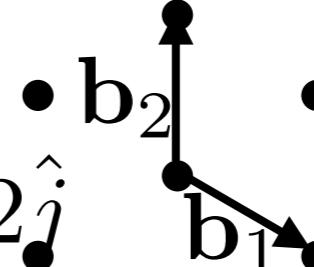
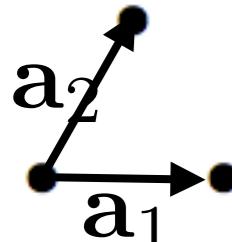
$$\mathbf{R} \cdot \mathbf{G} = ?$$

$$\mathbf{a}_1 = 3\hat{i}$$

$$\mathbf{a}_2 = 1.5\hat{i} + 2.6\hat{j}$$

$$\mathbf{b}_1 = 2.0944\hat{i} - 1.2092\hat{j}$$

$$\mathbf{b}_2 = 2.4184\hat{j}$$



Big Deal!!

$$\mathcal{E} \propto f_e(\theta) \left[\sum_{\mathbf{R}} e^{i\mathbf{R} \cdot \Delta\mathbf{k}} \right] \sum_{\mathbf{r}_p} f_{ap}(\theta) e^{i\mathbf{r}_p \cdot \Delta\mathbf{k}}$$

$$\mathbf{G} = \Delta\mathbf{k}$$

$$\mathbf{R} \cdot \mathbf{G} = ?$$

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

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

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