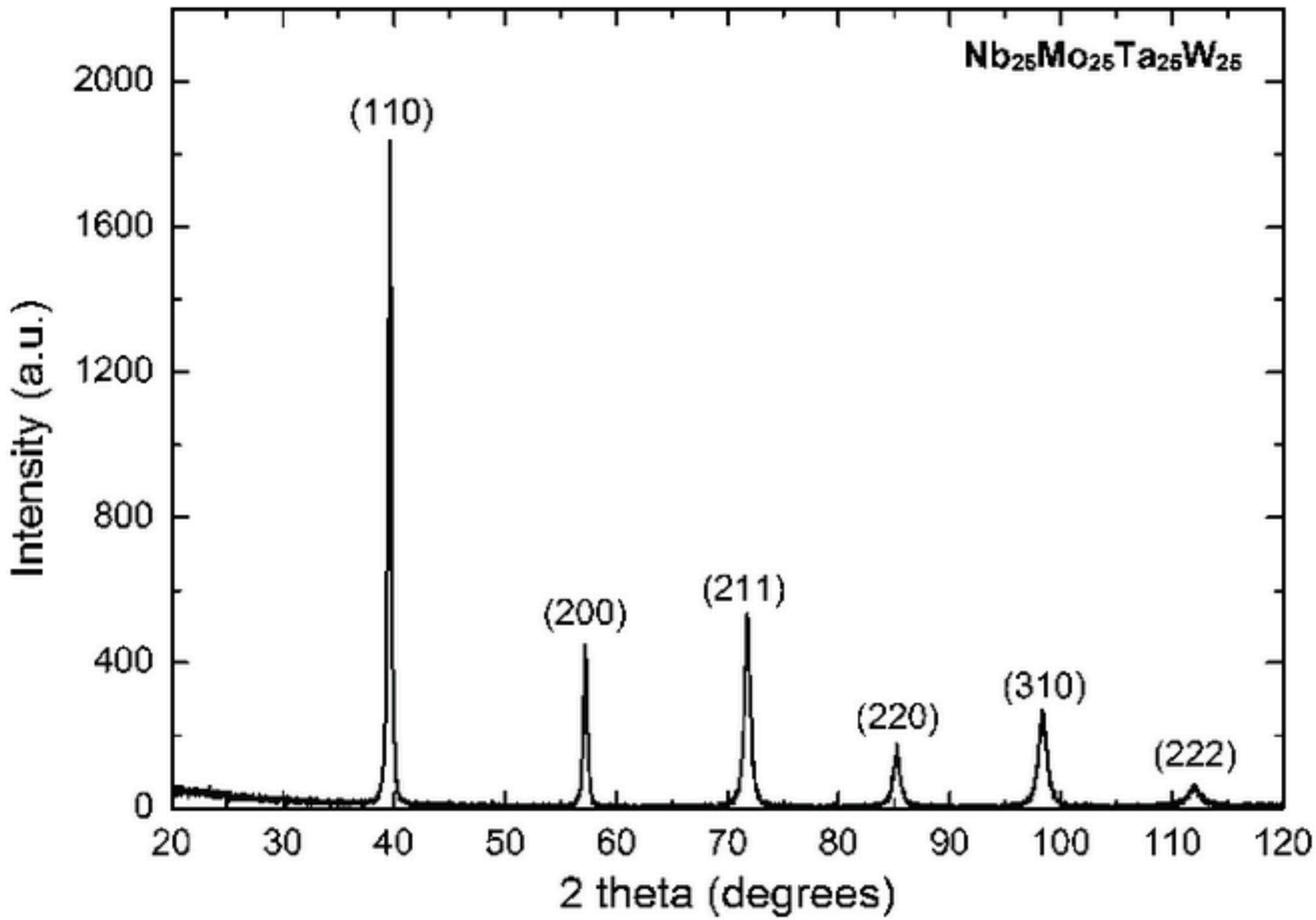


$Nb_{25}Mo_{25}Ta_{25}W_{25}$
(110)
(200)
(211)
(220)
(310)
(222)
Intensity (a.u.)
2 theta (degrees)
0
400
800
1200
1600
2000
20
30
40
50
60
70
80
90
100
110
120

Question #37

In Bragg's law, the key idea is that constructive interference occurs between reflected waves when:

A. the distance each reflected wave travels differs from the others by a whole wavelength (or two, or three...)
B. the reflected waves have the same amplitude.
C. the waves are reflected off planes of atoms
D. the angle of the incoming and outgoing waves is the same (law of reflection)
E. when the spacing between planes of atoms is the same as the wavelength of the x-rays

The angles at which Bragg peaks may occur depend on

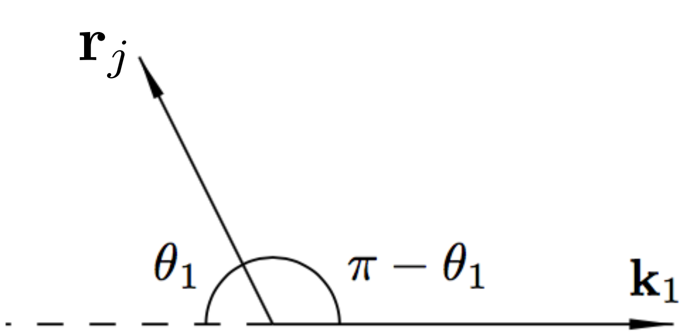
A. the spacing between planes of atoms
B.the spacing between atoms in the unit cell
C. whether or not the unit cell is conventional or primitive
D. the types of atoms in the unit cell
E. the spacing between planes of Bravais lattice points

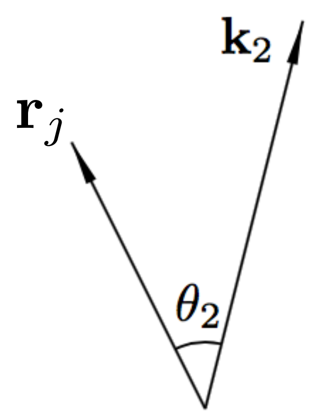
$$\mathcal{E}_1 \propto f_e(\theta)\frac{1}{r}e^{ikr-i\omega t} \qquad \boxed{1}$$

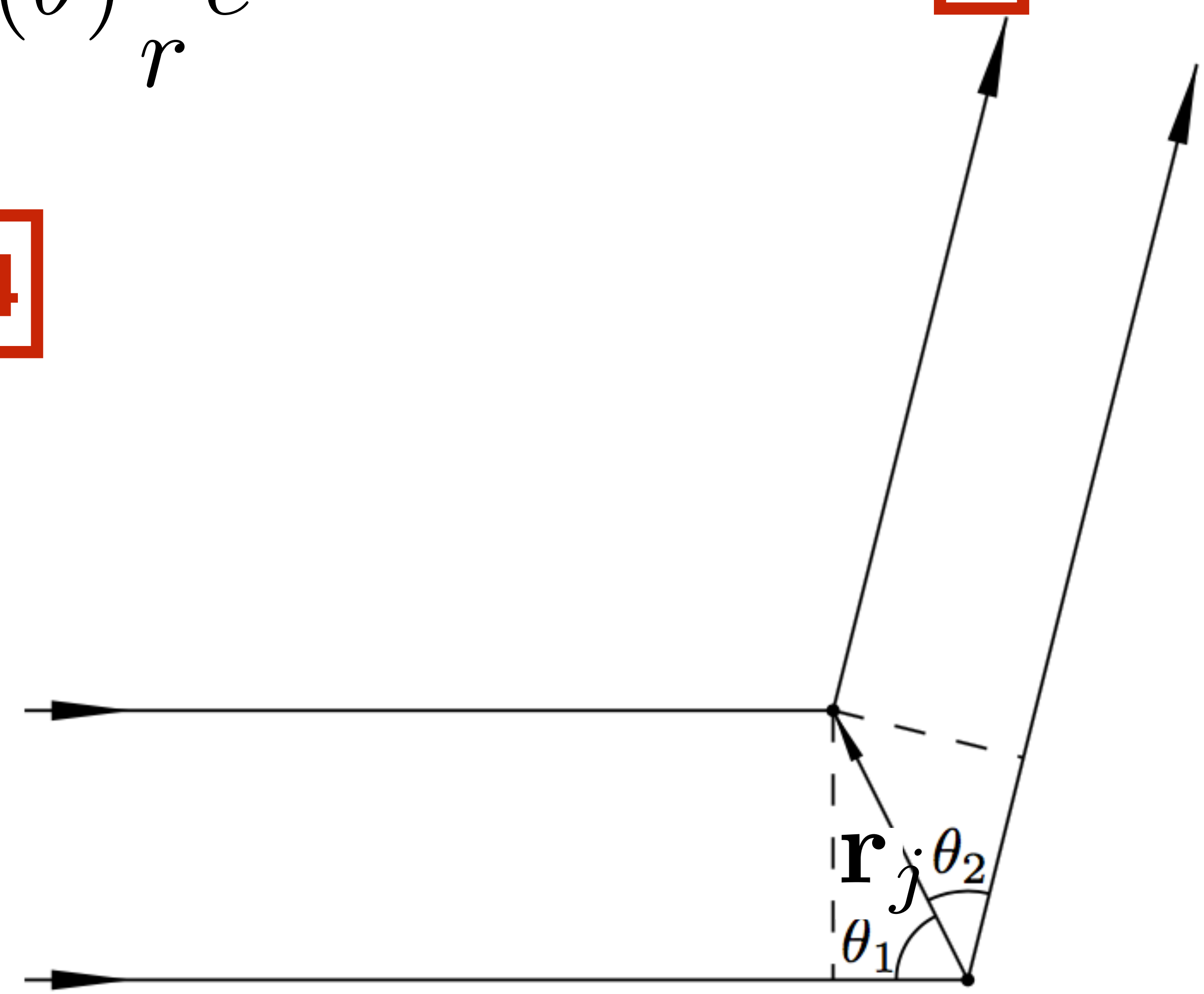
$$\mathcal{E}_2 \propto f_e(\theta)\frac{1}{r}e^{ikr-i\omega t+i\mathbf{r}_j\cdot\Delta\mathbf{k}} \qquad \boxed{2}$$

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

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







5 $$\mathcal{E} \propto f_e(\theta) \sum_j e^{i\mathbf{r_j}\cdot\Delta\mathbf{k}}$$

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

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

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

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

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

11 $$\mathcal{E} \propto f_e(\theta) \left[\sum_{\mathbf{R}} e^{i\mathbf{R}\cdot\Delta\mathbf{k}} \right] \sum_{\mathbf{r}_p} f_{ap}(\theta) e^{i\mathbf{r}_p\cdot\Delta\mathbf{k}}$$

12 $$f_{ap}(\theta) = \int \rho(\mathbf{r}_p + \mathbf{r}') e^{i\mathbf{r}'\cdot\Delta\mathbf{k}} d^3\mathbf{r}'$$

Big Deal!!

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

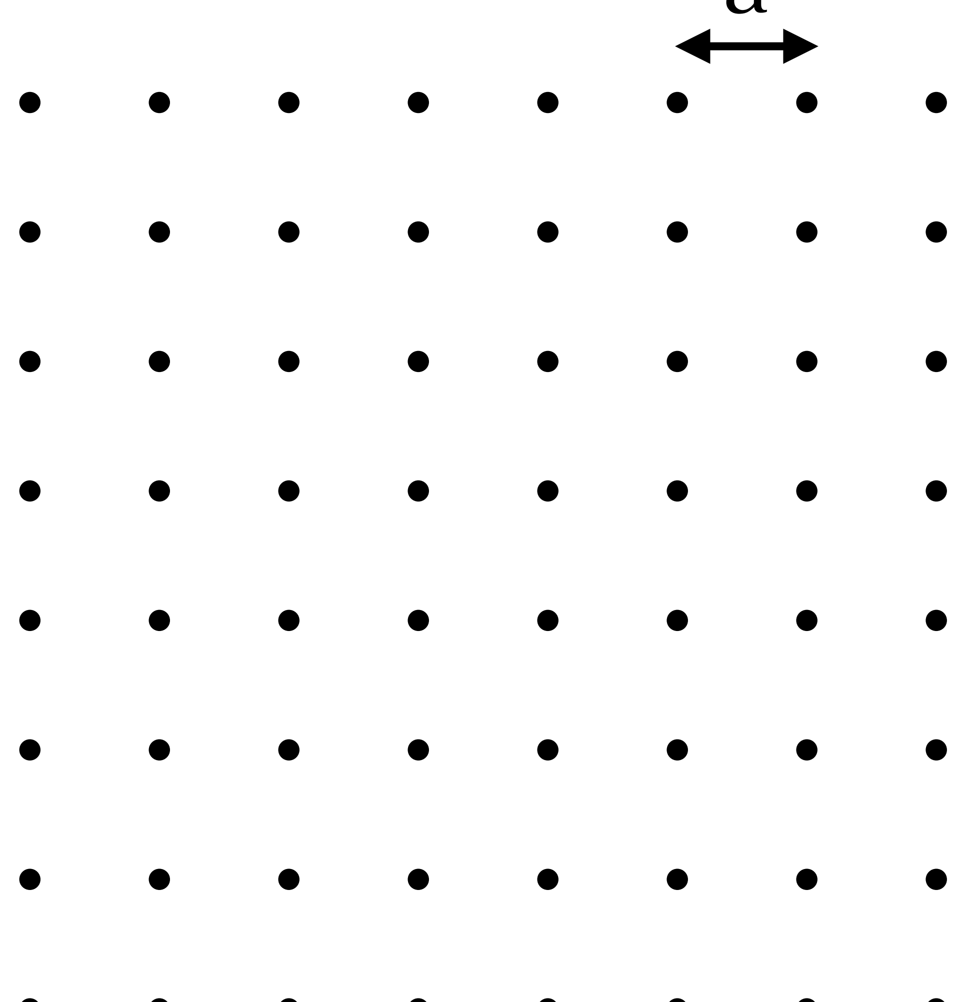
$$\mathbf{G} = \Delta\mathbf{k}$$

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

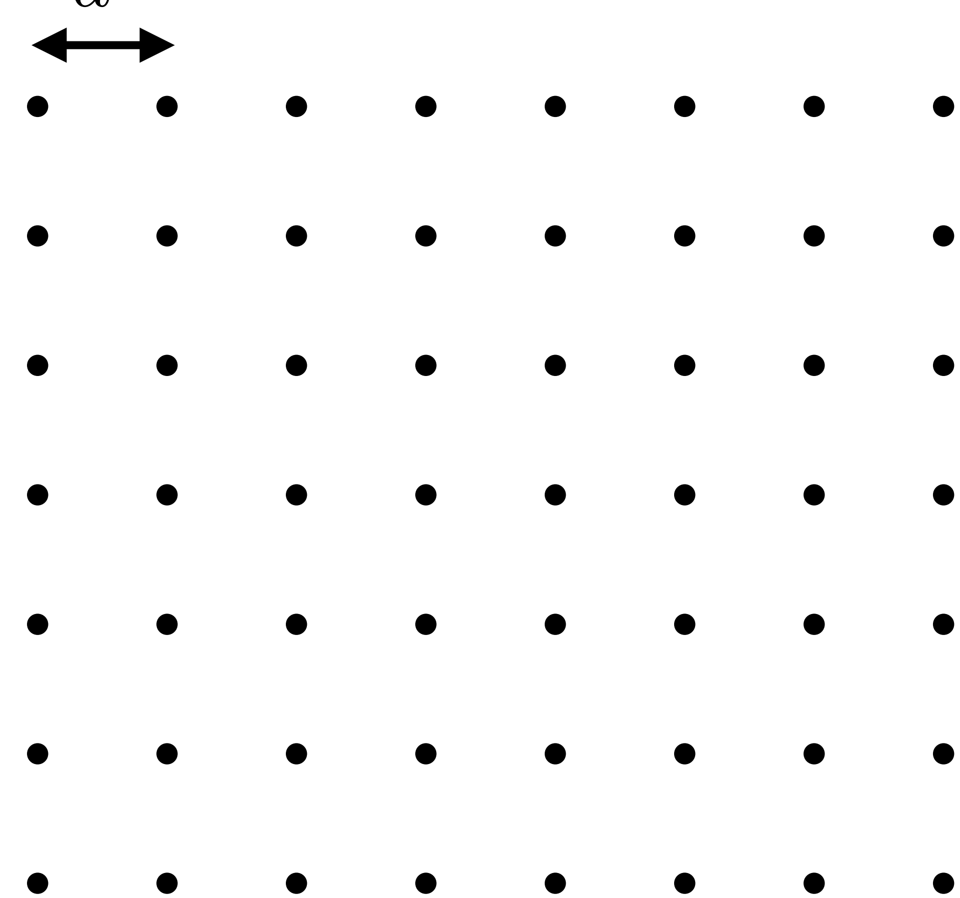
Big Deal!!

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

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

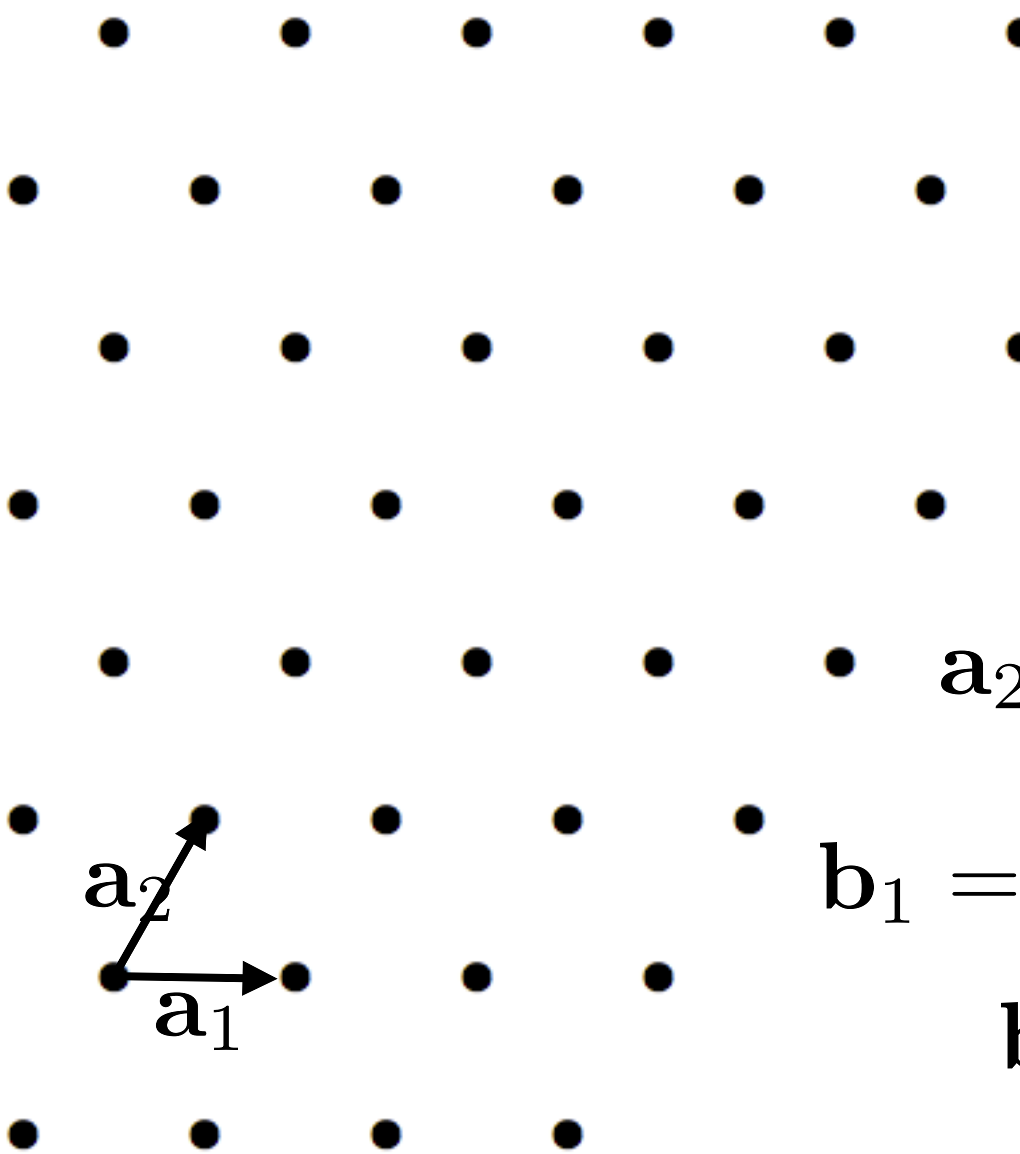


$$\mathbf{R}\cdot\mathbf{G} = ?$$



Big Deal!!

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



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

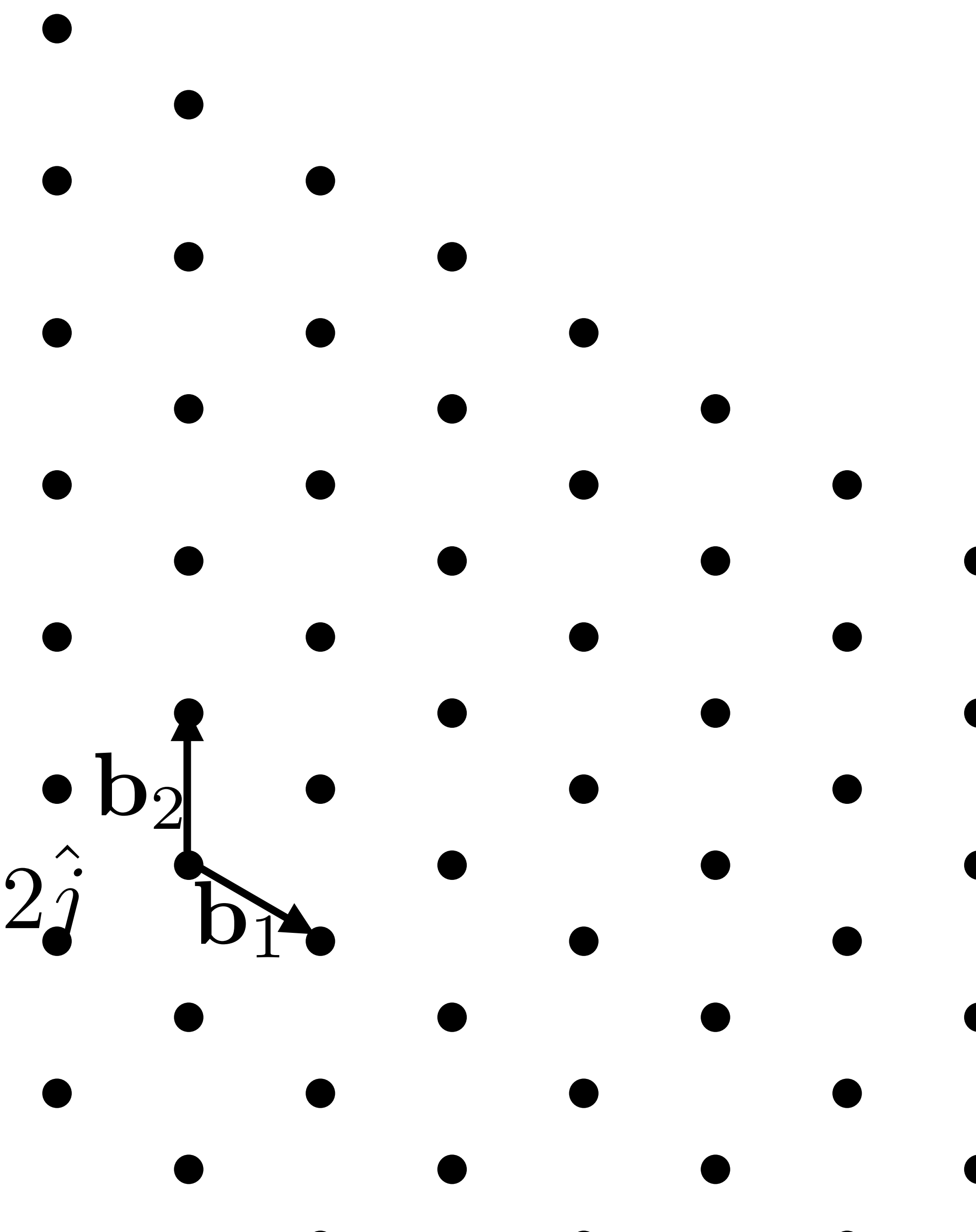
$$\mathbf{R}\cdot\mathbf{G} = ?$$

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

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

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

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



Big Deal!!

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

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

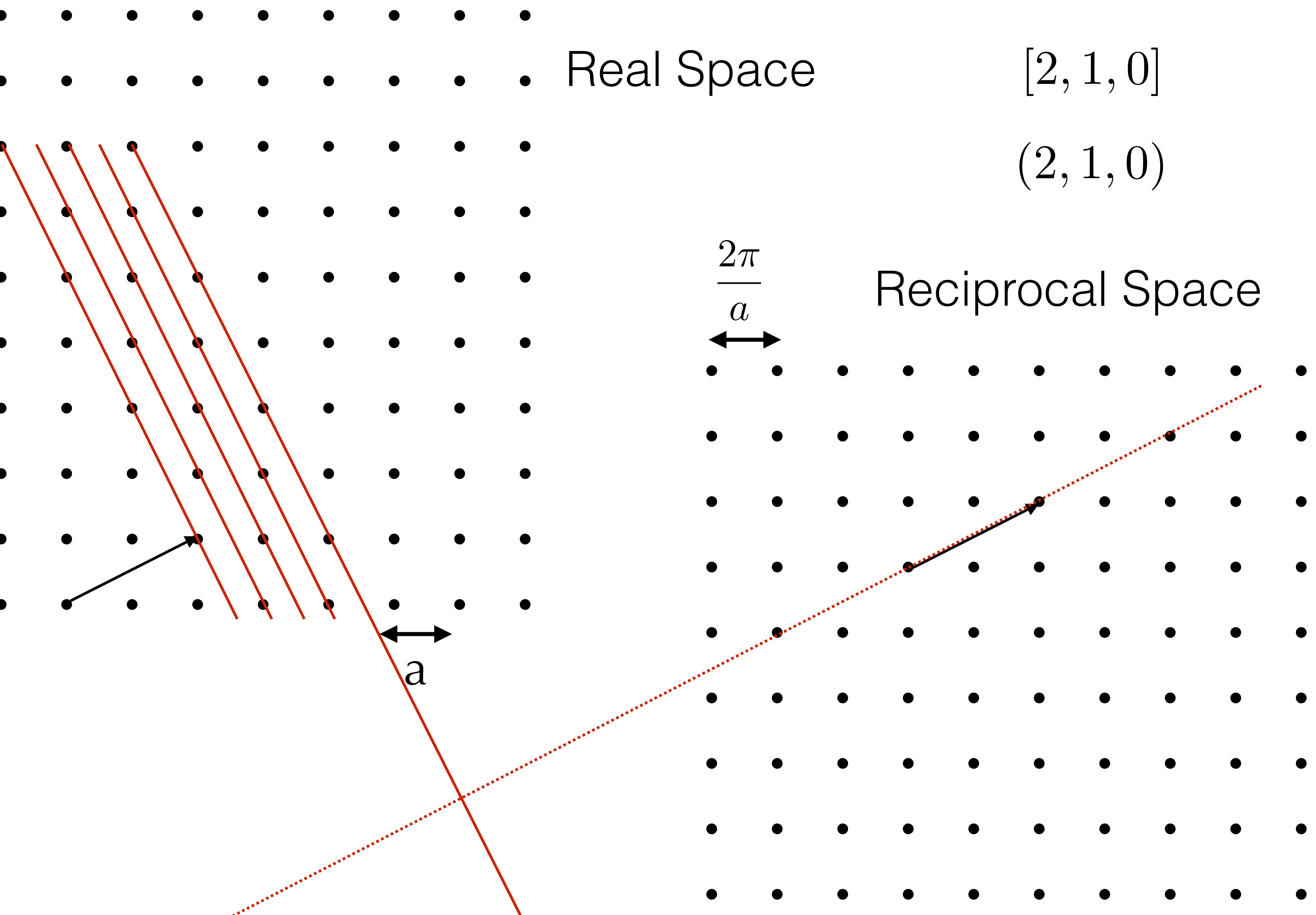
$$\mathbf{R}\cdot\mathbf{G} = ?$$

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

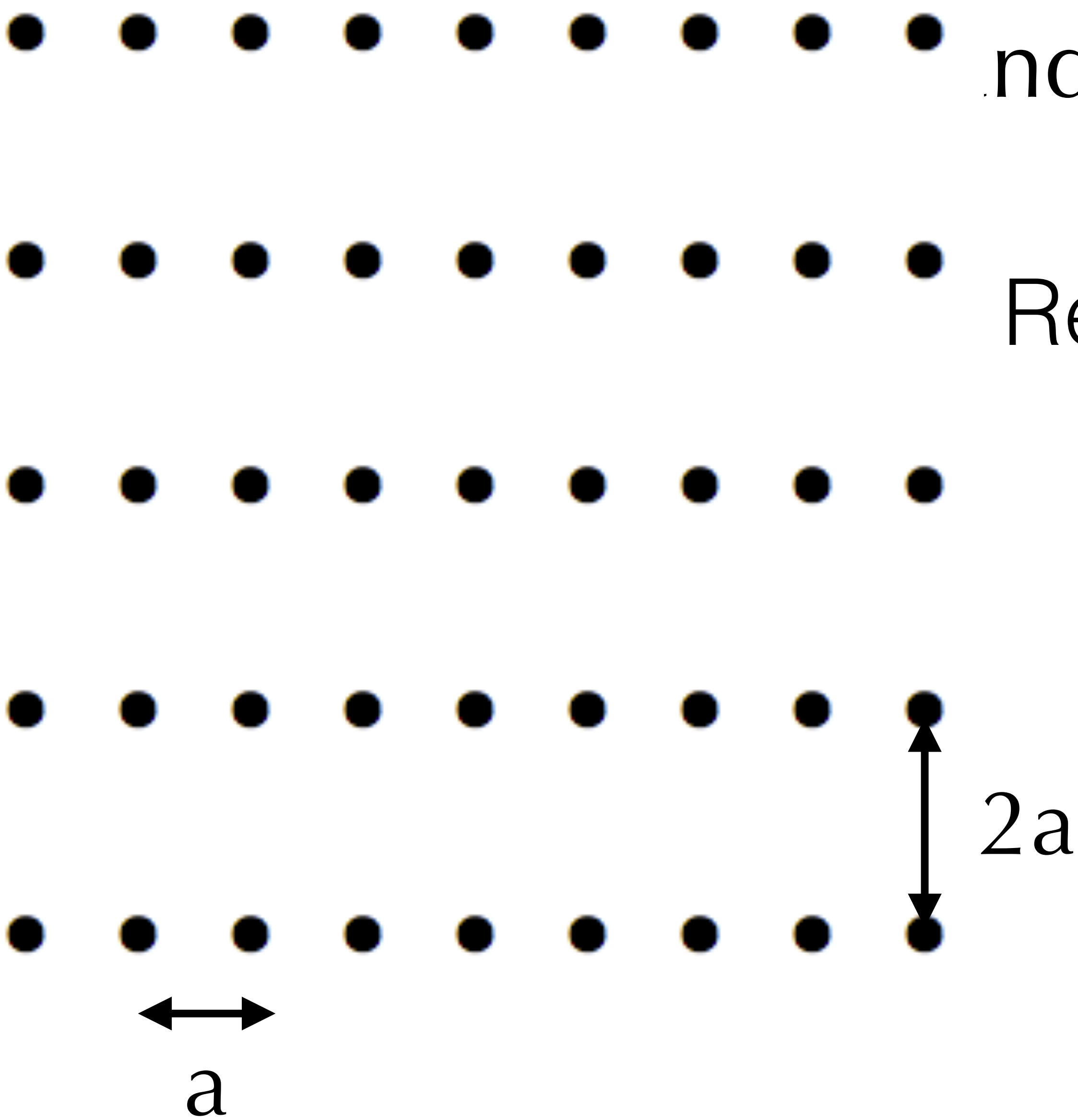
$$\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)}$$

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

Planes and directions revisited



nd directions revisited

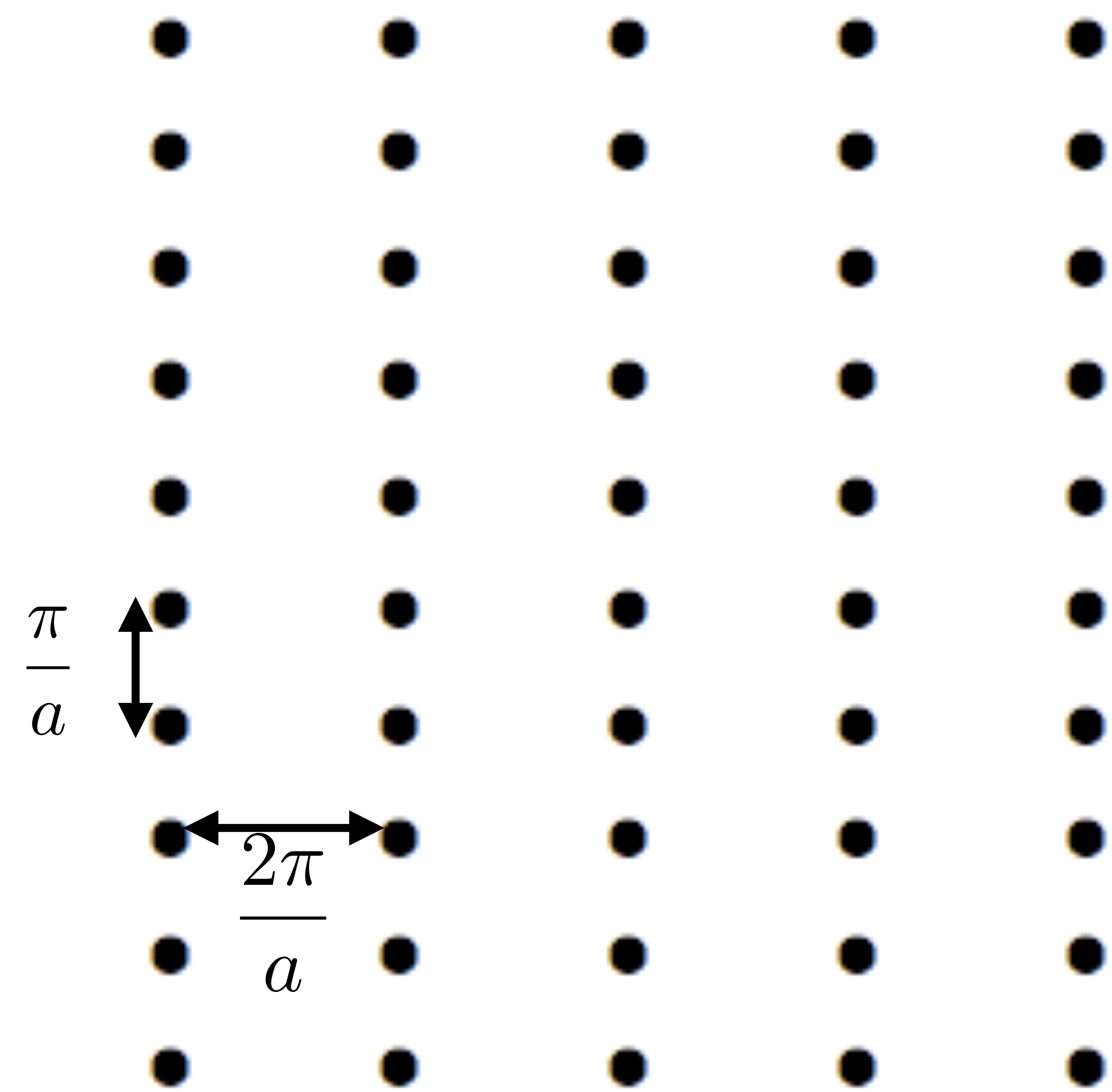


Real Space $[2, 1, 0]$

(h, k, l)

$(2, 1, 0)$

Reciprocal Space

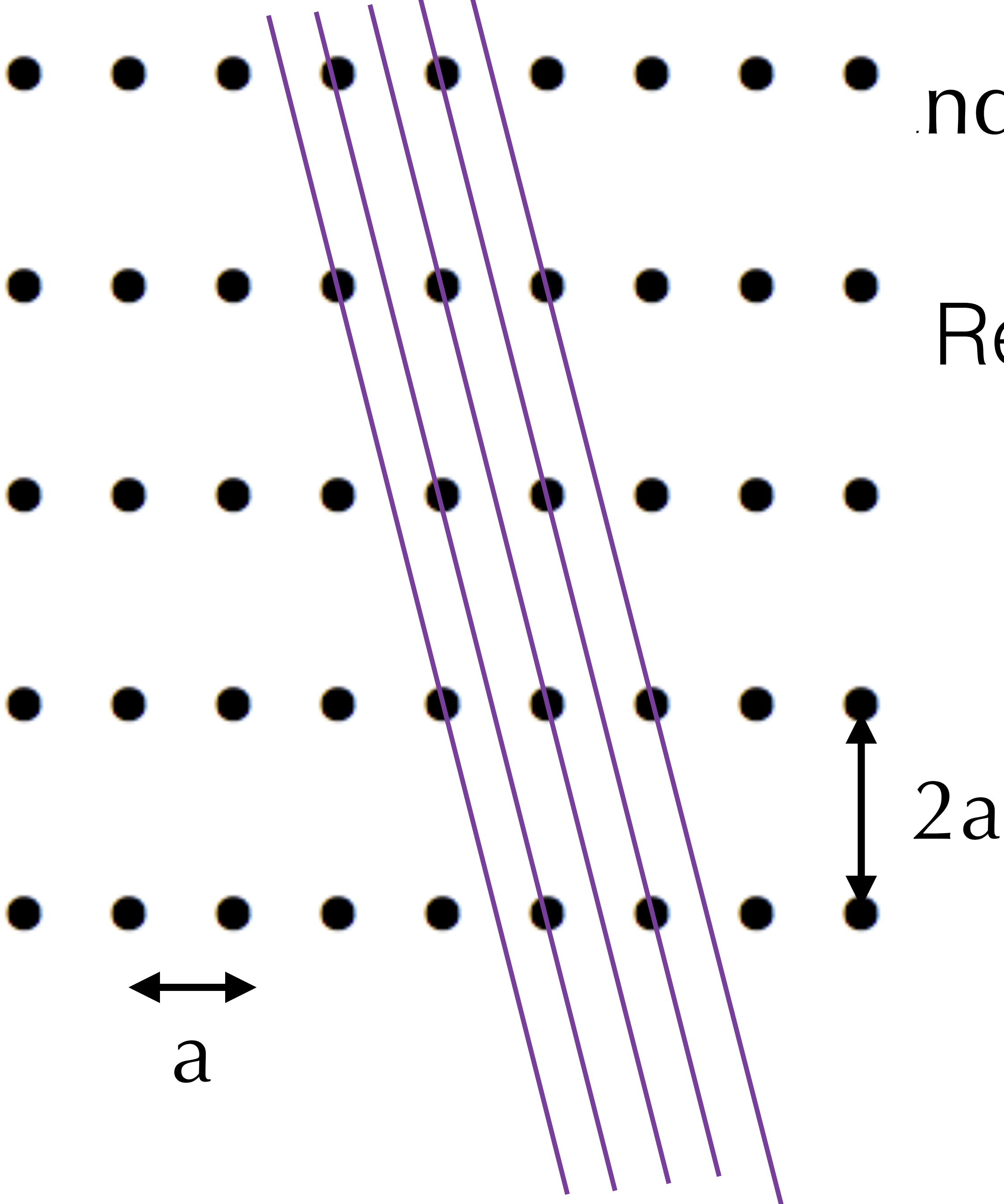


$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

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

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

nd directions revisited

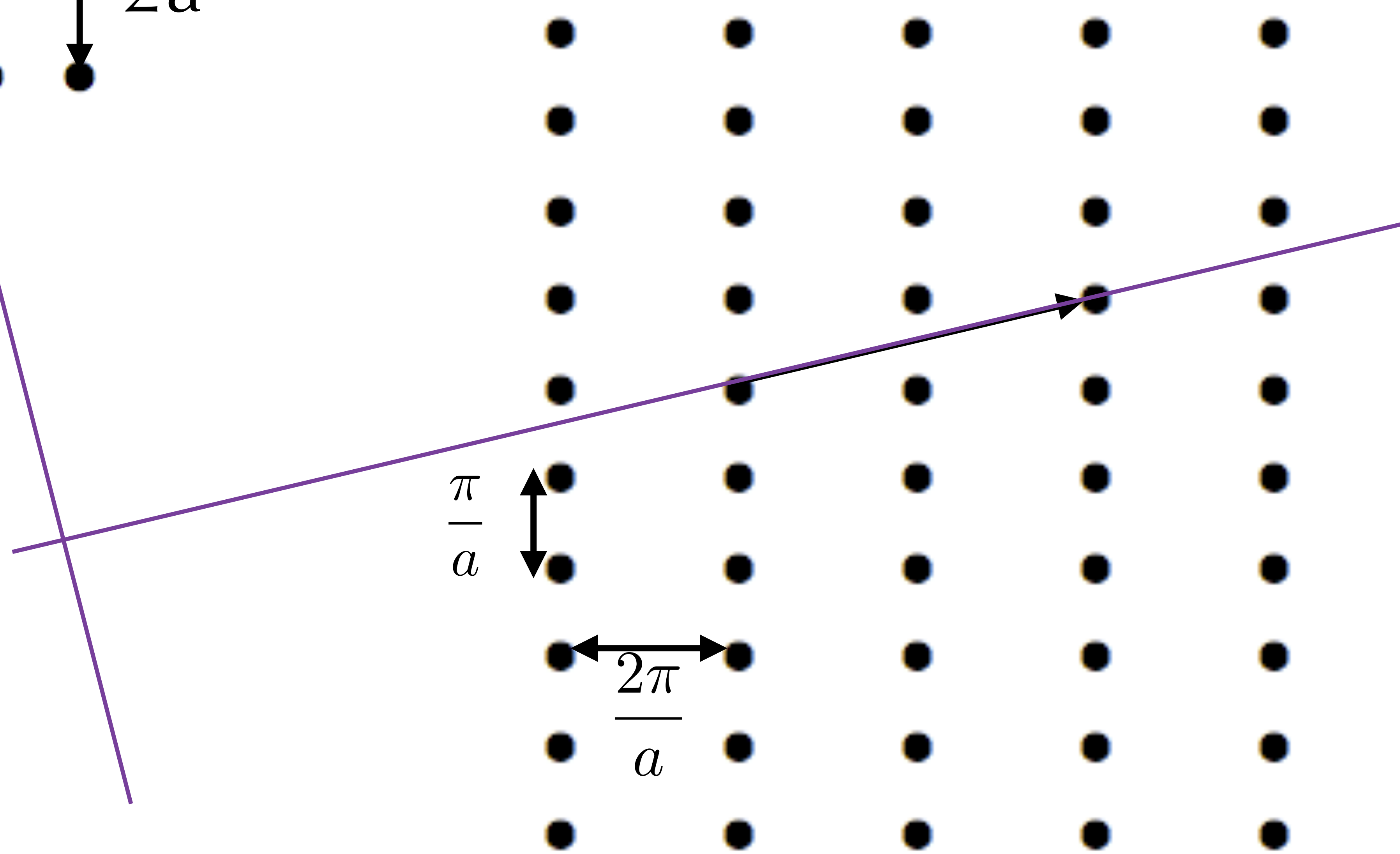


Real Space $[2, 1, 0]$

(h, k, l)

$(2, 1, 0)$

Reciprocal Space

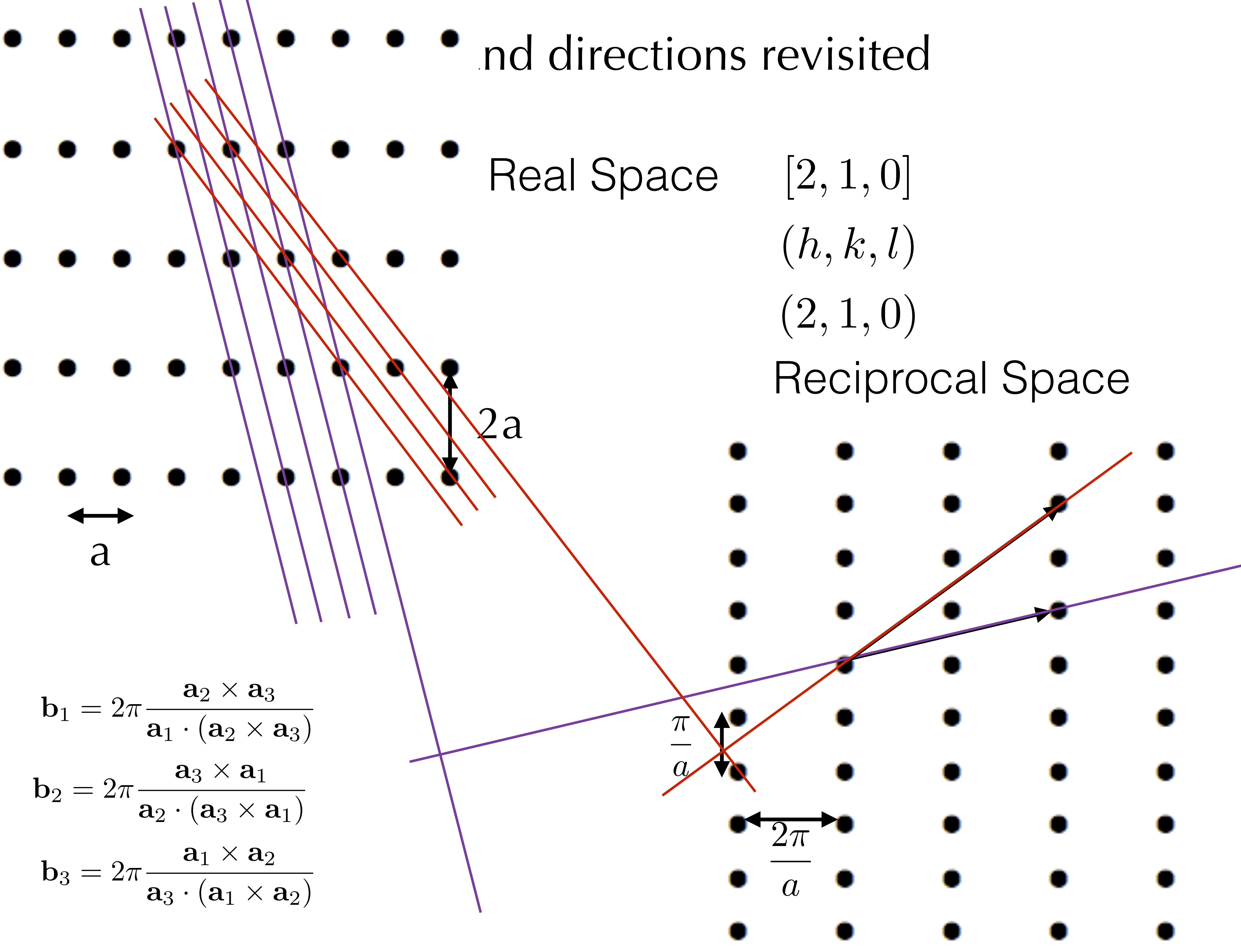


$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

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

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

nd directions revisited



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

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

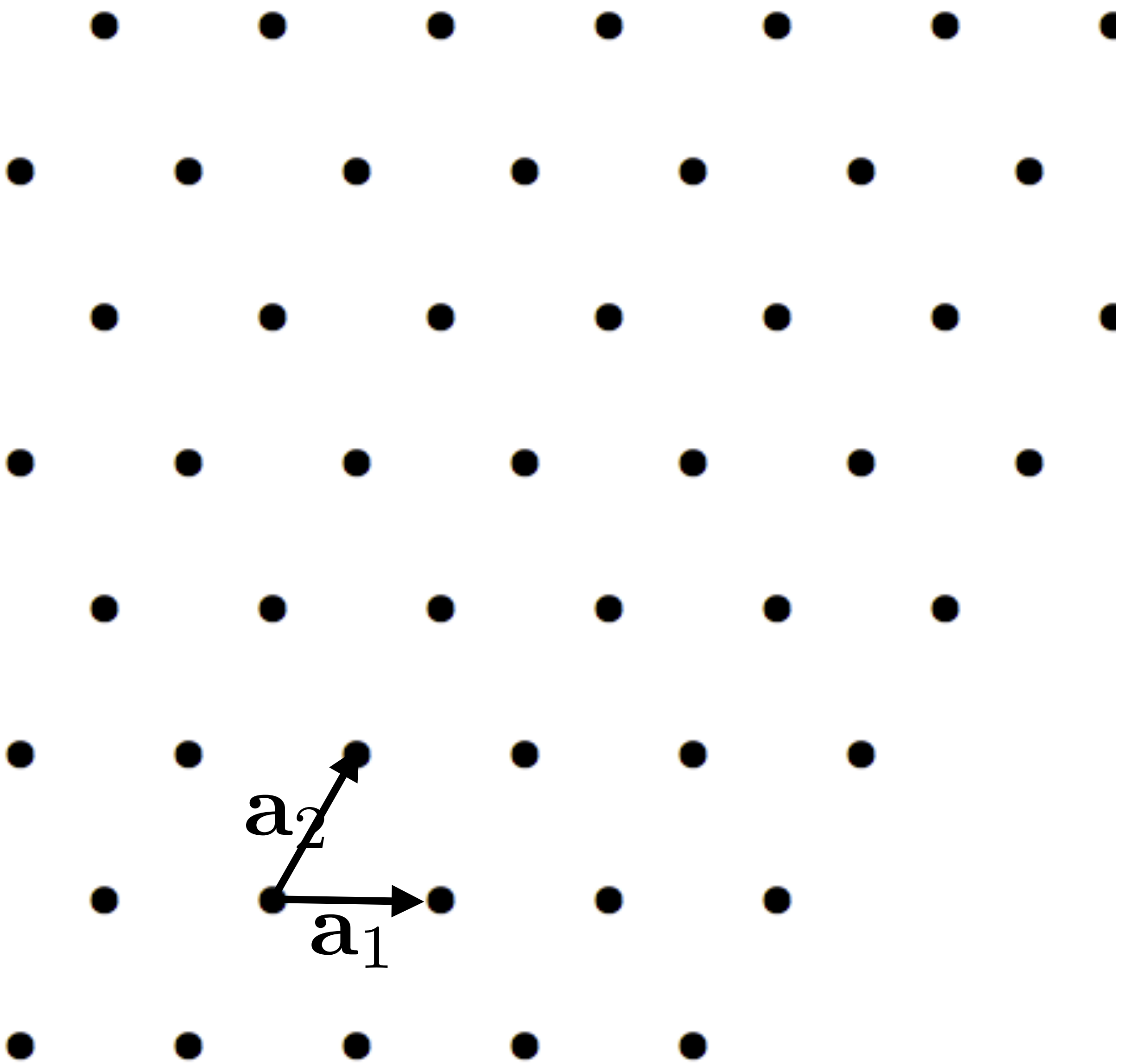
$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)}$$

You try one!!

$$(2, 1, 0)$$

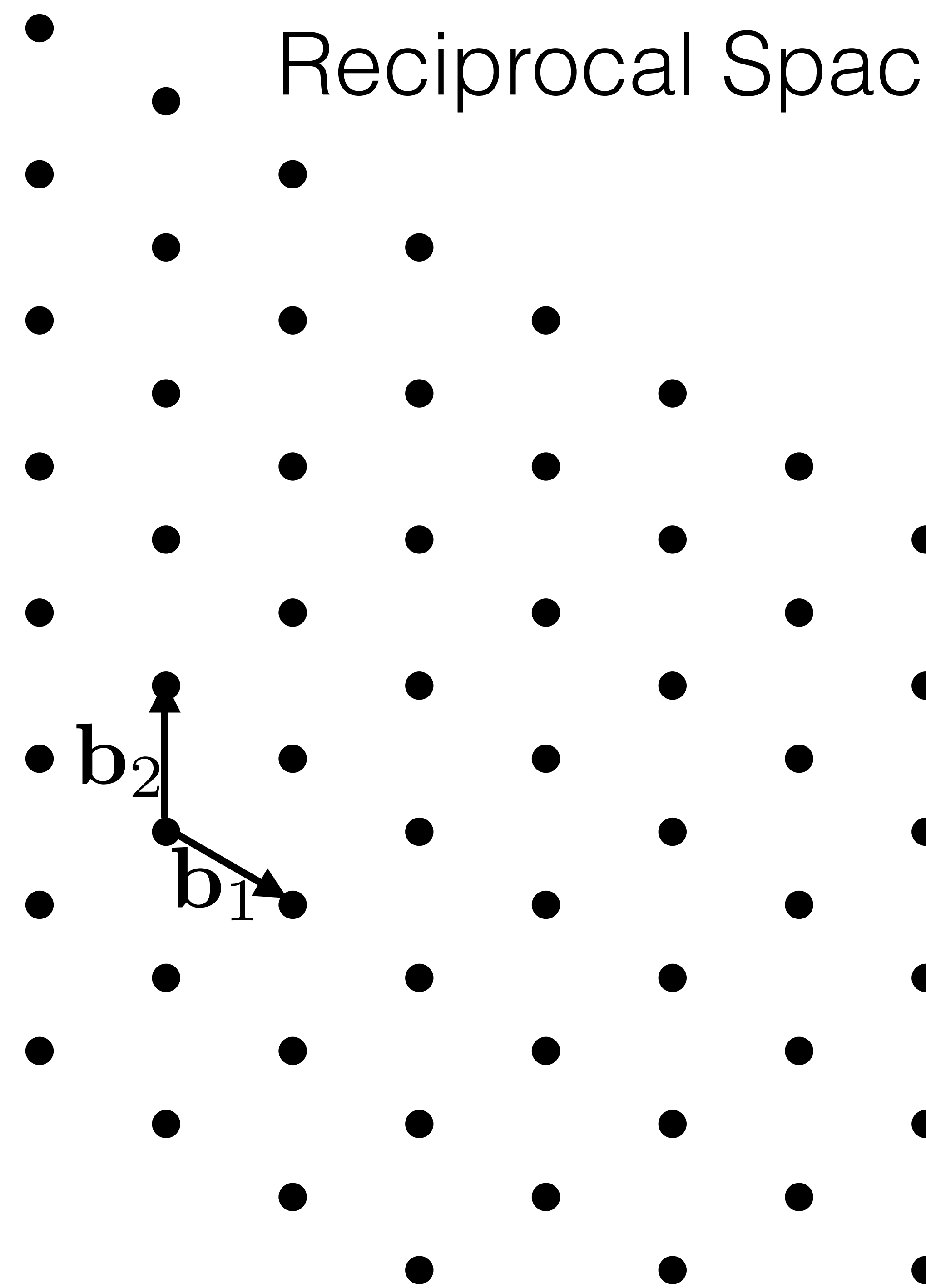
$$(2, 3, 0)$$

Real Space



$$\frac{A}{h}, \frac{A}{k}, \frac{A}{l}$$

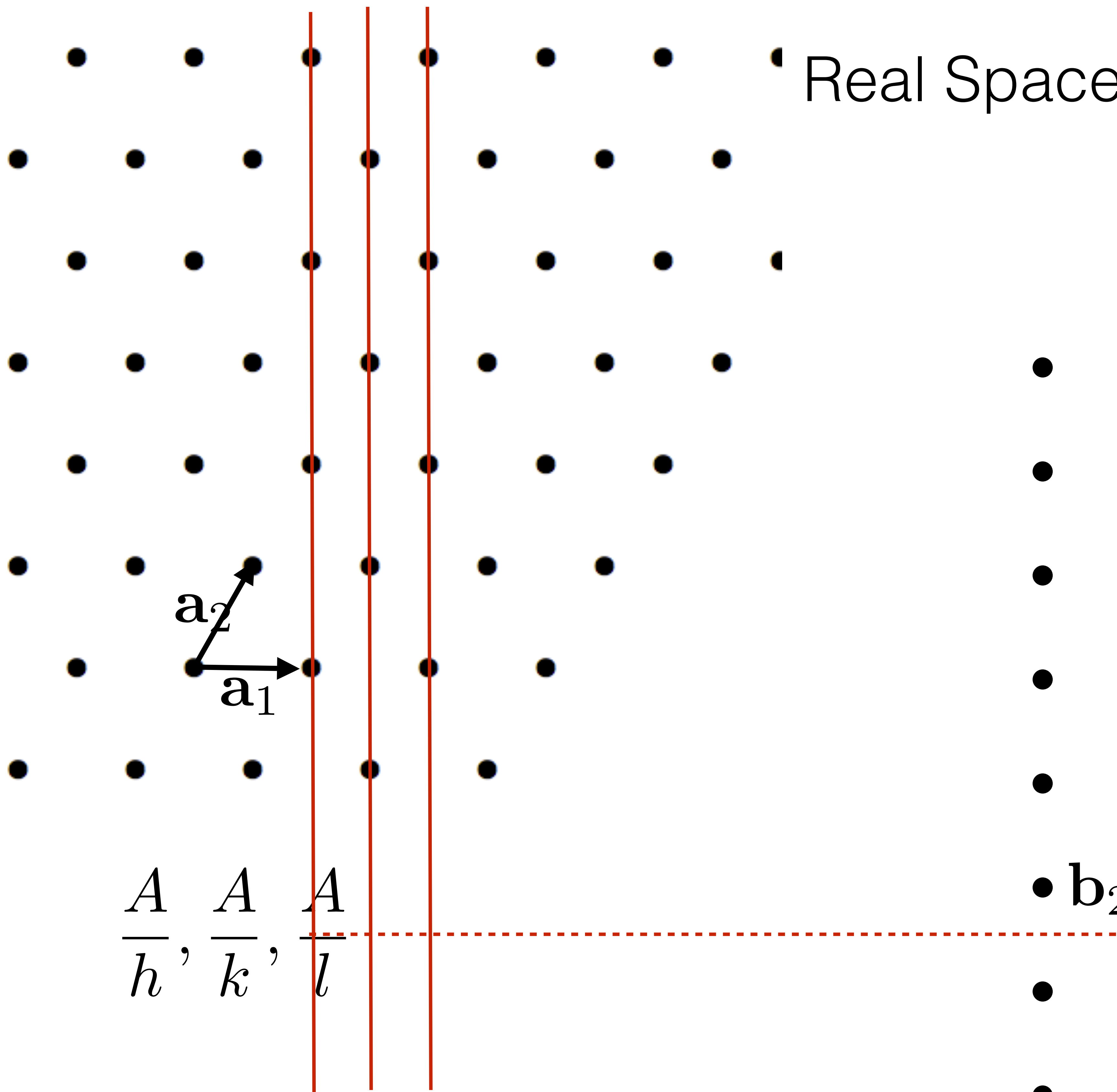
Reciprocal Space

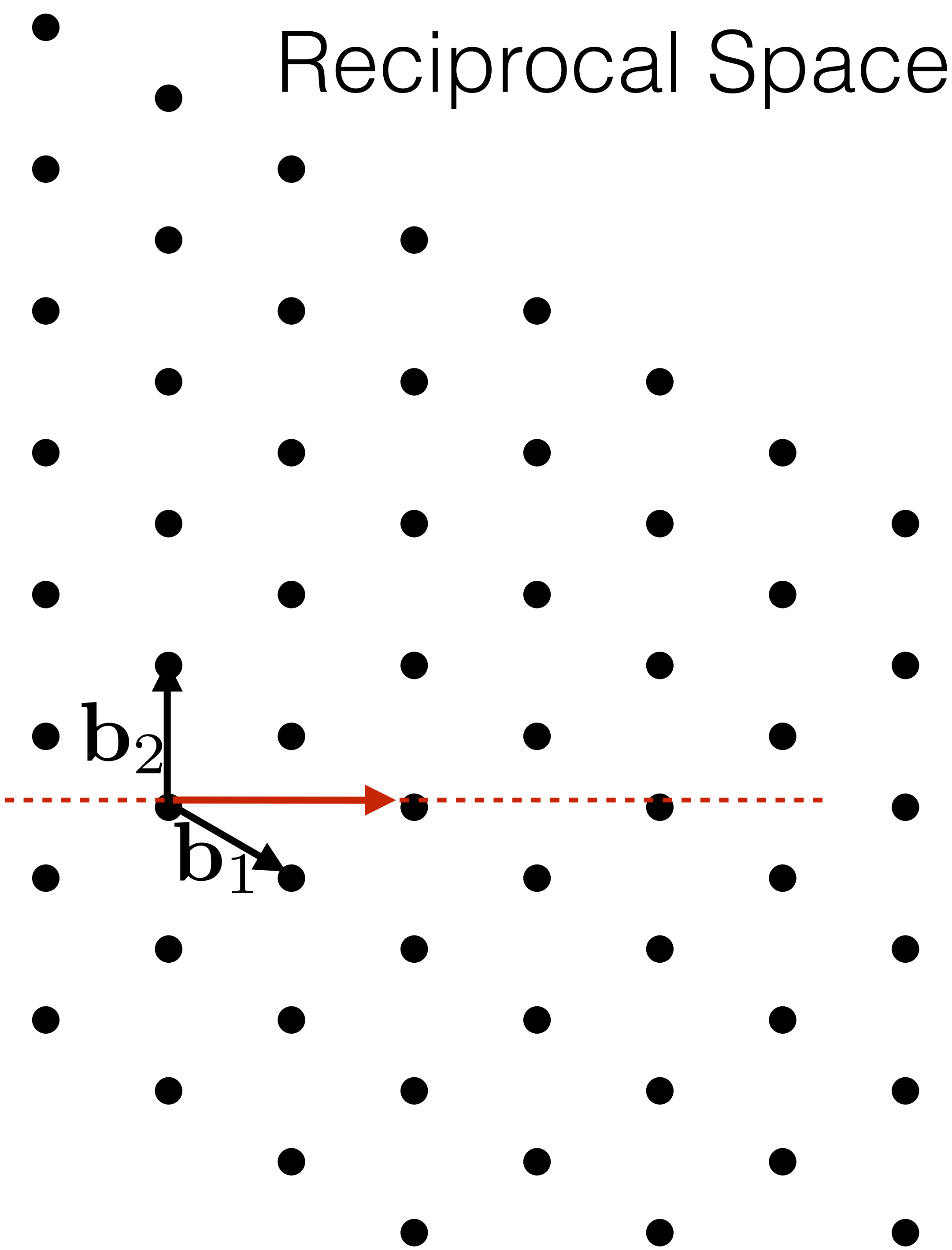


You try one!!

$$(2, 1, 0)$$

$$(2, 3, 0)$$

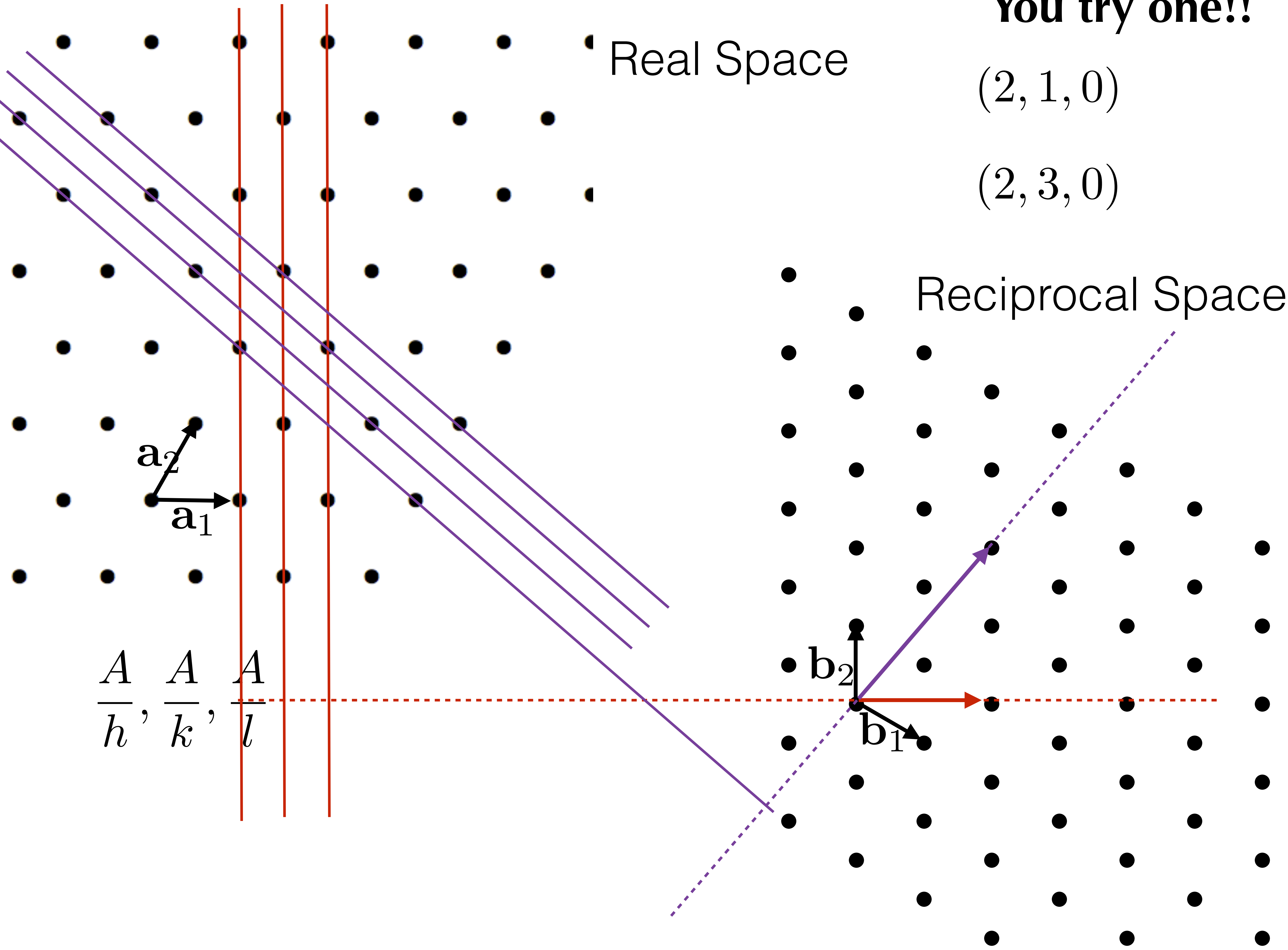




You try one!!

$(2, 1, 0)$

$(2, 3, 0)$



Which of the following is a real-space lattice vector for a copper crystal?

A. $4\pi/a(\hat{\imath}+\hat{\jmath}+\hat{k})$

B. $4\pi/a(\hat{\imath}/2+\hat{\jmath}/2+\hat{k}/2)$

C. $4\pi/a(\hat{\imath}+\hat{\jmath}/2+\hat{k}/2)$

D. $a(\hat{\imath}/2+\hat{\jmath}/2+\hat{k}/2)$

E. $a(\hat{\imath}+\hat{\jmath}/2+\hat{k}/2)$

Question #40

Which of the following is a reciprocal lattice vector for a copper crystal?

A. $4\pi/a(\hat{\imath}/2+\hat{\jmath}/2+\hat{k}/2)$

B. $4\pi/a(\hat{\imath}+\hat{\jmath}+\hat{k})$

C. $4\pi/a(\hat{\imath}+\hat{\jmath}/2+\hat{k}/2)$

D. $a(\hat{\imath}/2+\hat{\jmath}/2+\hat{k}/2)$

E. $a(\hat{\imath}+\hat{\jmath}/2+\hat{k}/2)$

Question #40

Which of the following is a reciprocal lattice vector for a copper crystal?

A. $4\pi/a(\hat{\imath}/2+\hat{\jmath}/2+\hat{k}/2)$

B. $4\pi/a(\hat{\imath}+\hat{\jmath}+\hat{k})$

C. $4\pi/a(\hat{\imath}+\hat{\jmath}/2+\hat{k}/2)$

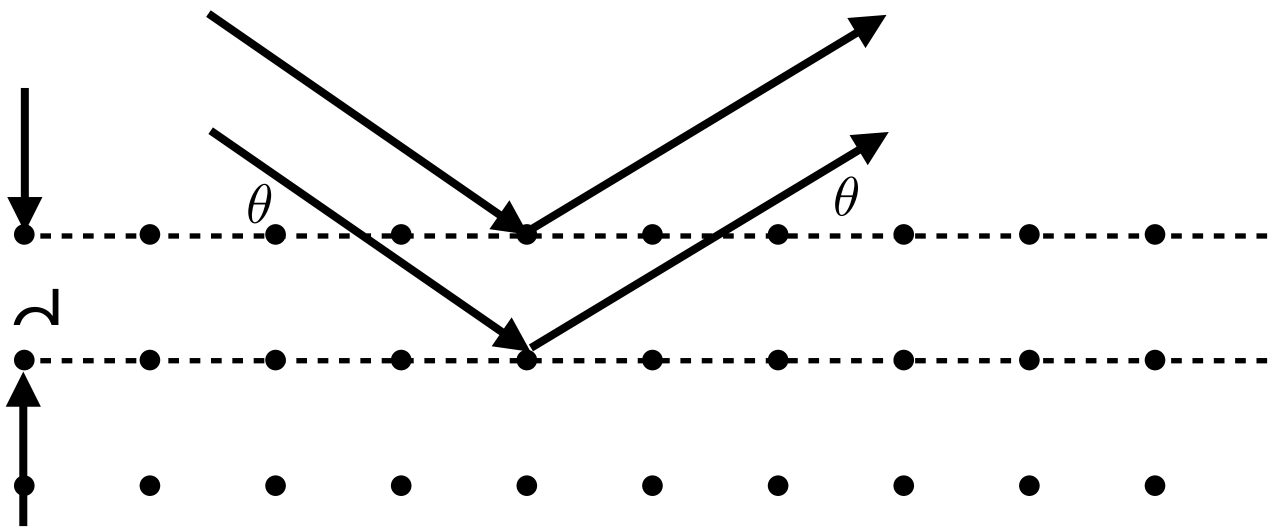
D. $a(\hat{\imath}/2+\hat{\jmath}/2+\hat{k}/2)$

E. $a(\hat{\imath}+\hat{\jmath}/2+\hat{k}/2)$

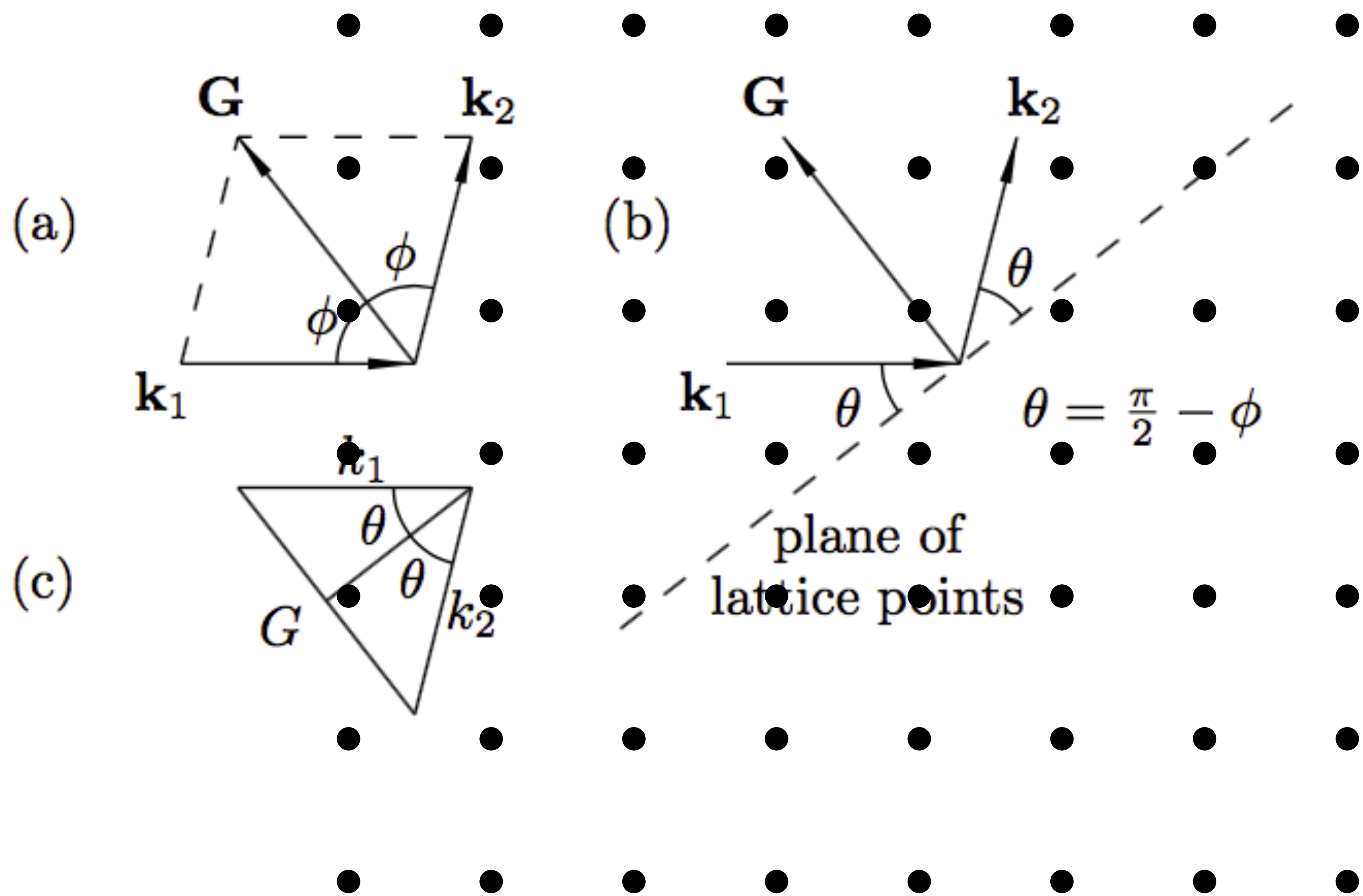
$$\mathbf{b}_1 = 2\pi\frac{\mathbf{a}_2\times\mathbf{a}_3}{\mathbf{a}_1\cdot(\mathbf{a}_2\times\mathbf{a}_3)}$$

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

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



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



$$G = 2k\sin\theta$$

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

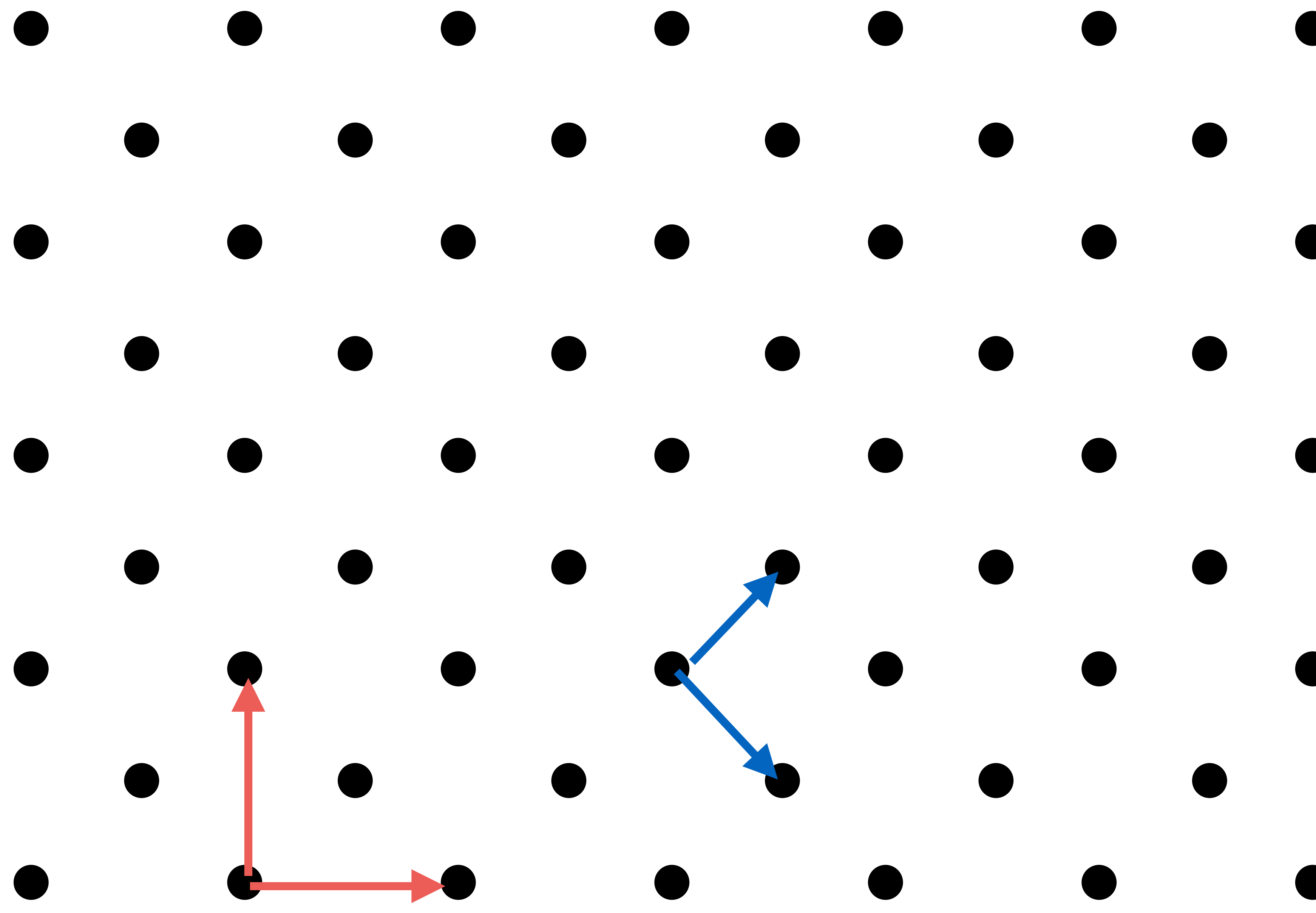
$$\lambda = 1.542 \text{ Å}$$

$$a = 3.61 \text{ Å}$$

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

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

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



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

$$\lambda = 1.542 \text{ Å}$$

$$a = 3.61 \text{ Å}$$

h

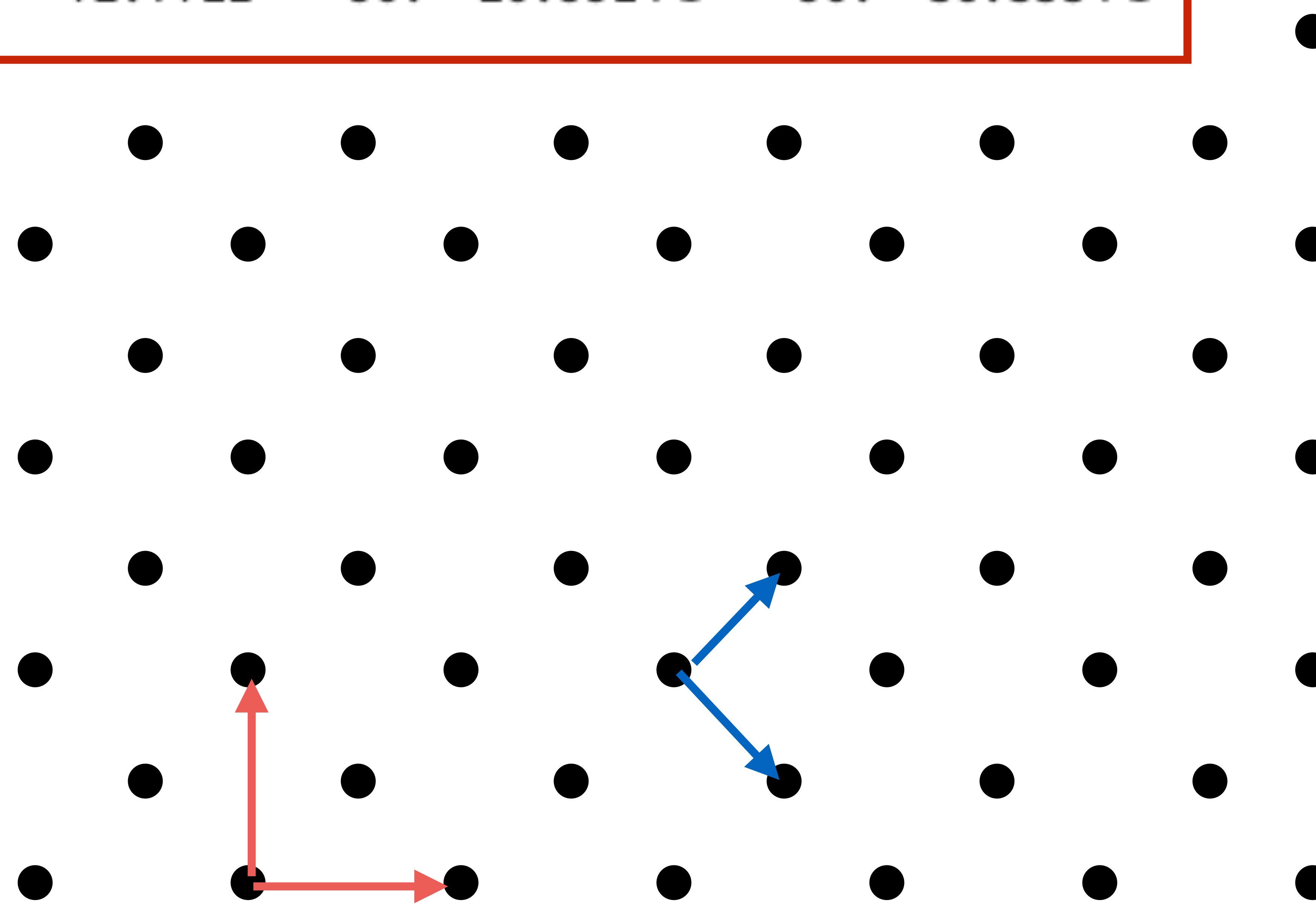
k

0.	12.3318	25.2866	39.8455	58.6818
12.3318	17.5801	28.5265	42.4835	61.7131
25.2866	28.5265	37.1624	50.3584	72.7711
39.8455	42.4835	50.3584	64.9739	90. − 20.9914 i
58.6818	61.7131	72.7711	90. − 20.9914 i	90. − 36.3554 i

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

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

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



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

$$\lambda = 1.542 \text{ Å}$$

$$a = 3.61 \text{ Å}$$

h ↓ k →

0.	12.3318	25.2866	39.8455	58.6818
12.3318	17.5801	28.5265	42.4835	61.7131
25.2866	28.5265	37.1624	50.3584	72.7711
39.8455	42.4835	50.3584	64.9739	90. - 20.9914 i
58.6818	61.7131	72.7711	90. - 20.9914 i	90. - 36.3554 i

h ↓ k →

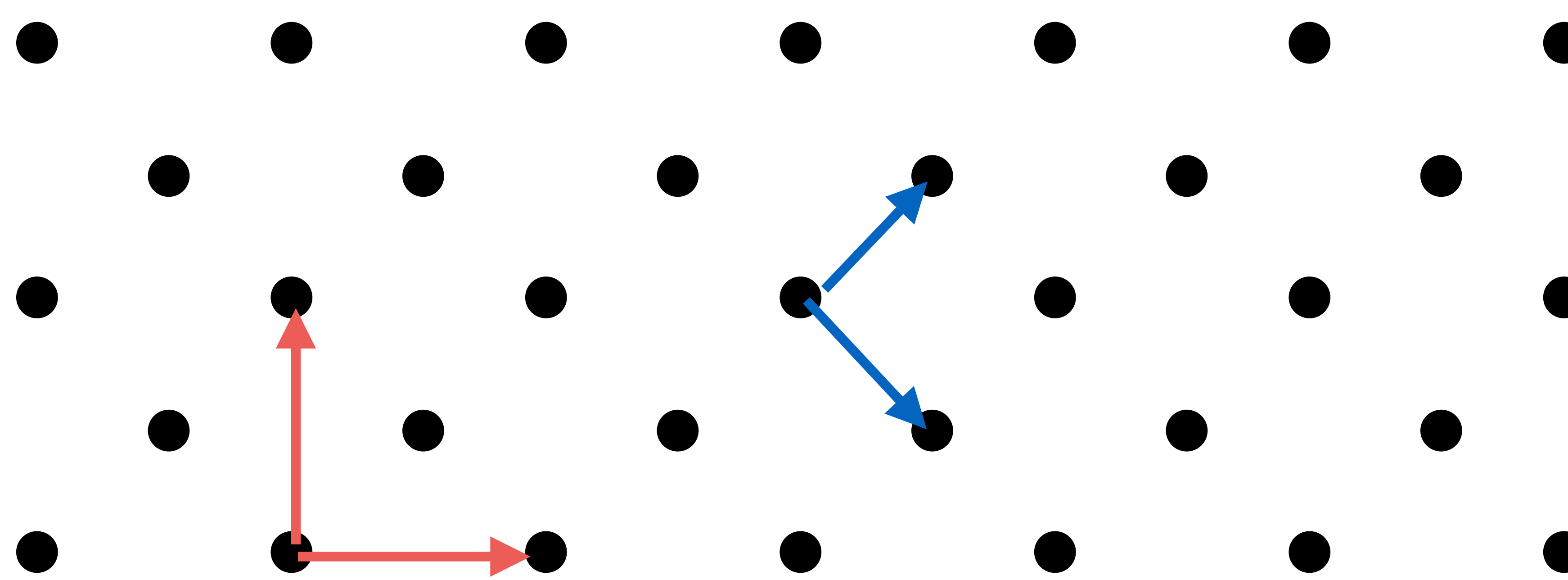
TableForm=

0.	17.5801	37.1624	64.9739	90. - 36.3554 i
17.5801	25.2866	42.4835	72.7711	90. - 39.3563 i
37.1624	42.4835	58.6818	90. - 23.9993 i	90. - 46.6866 i
64.9739	72.7711	90. - 23.9993 i	90. - 42.0372 i	90. - 55.662 i
90. - 36.3554 i	90. - 39.3563 i	90. - 46.6866 i	90. - 55.662 i	90. - 64.7129 i

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

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

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



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

$$\lambda = 1.542\ \text{Å}$$

$$a = 3.61\ \text{Å}$$

h

k

0.	~~12.3318~~	25.2866	~~39.8455~~	58.6818
~~12.3318~~	17.5801	~~28.5265~~	42.4835	~~61.7131~~
25.2866	~~28.5265~~	37.1624	~~50.3584~~	72.7711
~~39.8455~~	42.4835	~~50.3584~~	64.9739	90. − 20.9914 i
58.6818	~~61.7131~~	72.7711	90. − 20.9914 i	90. − 36.3554 i

h

TableForm=

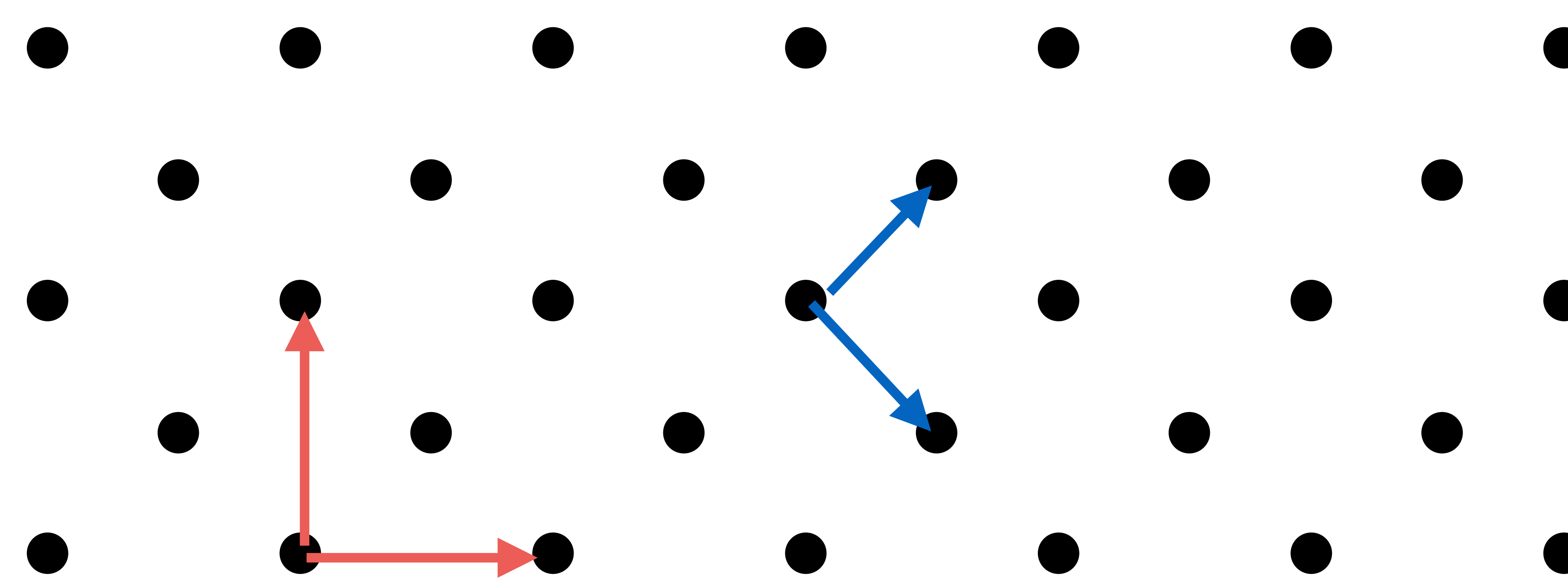
k

0.	17.5801	37.1624	64.9739	90. − 36.3554 i
17.5801	25.2866	42.4835	72.7711	90. − 39.3563 i
37.1624	42.4835	58.6818	90. − 23.9993 i	90. − 46.6866 i
64.9739	72.7711	90. − 23.9993 i	90. − 42.0372 i	90. − 55.662 i
90. − 36.3554 i	90. − 39.3563 i	90. − 46.6866 i	90. − 55.662 i	90. − 64.7129 i

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

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

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



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

$\lambda = 1.542$ Å

$a = 3.61$ Å

h ↓, k →

0.	~~12.3318~~	25.2866	~~39.8455~~	58.6818
~~12.3318~~	17.5801	~~28.5265~~	42.4835	~~61.7131~~
25.2866	~~28.5265~~	37.1624	~~50.3584~~	72.7711
~~39.8455~~	42.4835	~~50.3584~~	64.9739	90. − 20.9914 i
58.6818	~~61.7131~~	72.7711	90. − 20.9914 i	90. − 36.3554 i

h ↓, k →

TableForm=

0.	17.5801	37.1624	64.9739	90. − 36.3554 i
17.5801	25.2866	42.4835	72.7711	90. − 39.3563 i
37.1624	42.4835	58.6818	90. − 23.9993 i	90. − 46.6866 i
64.9739	72.7711	90. − 23.9993 i	90. − 42.0372 i	90. − 55.662 i
90. − 36.3554 i	90. − 39.3563 i	90. − 46.6866 i	90. − 55.662 i	90. − 64.7129 i

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

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

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