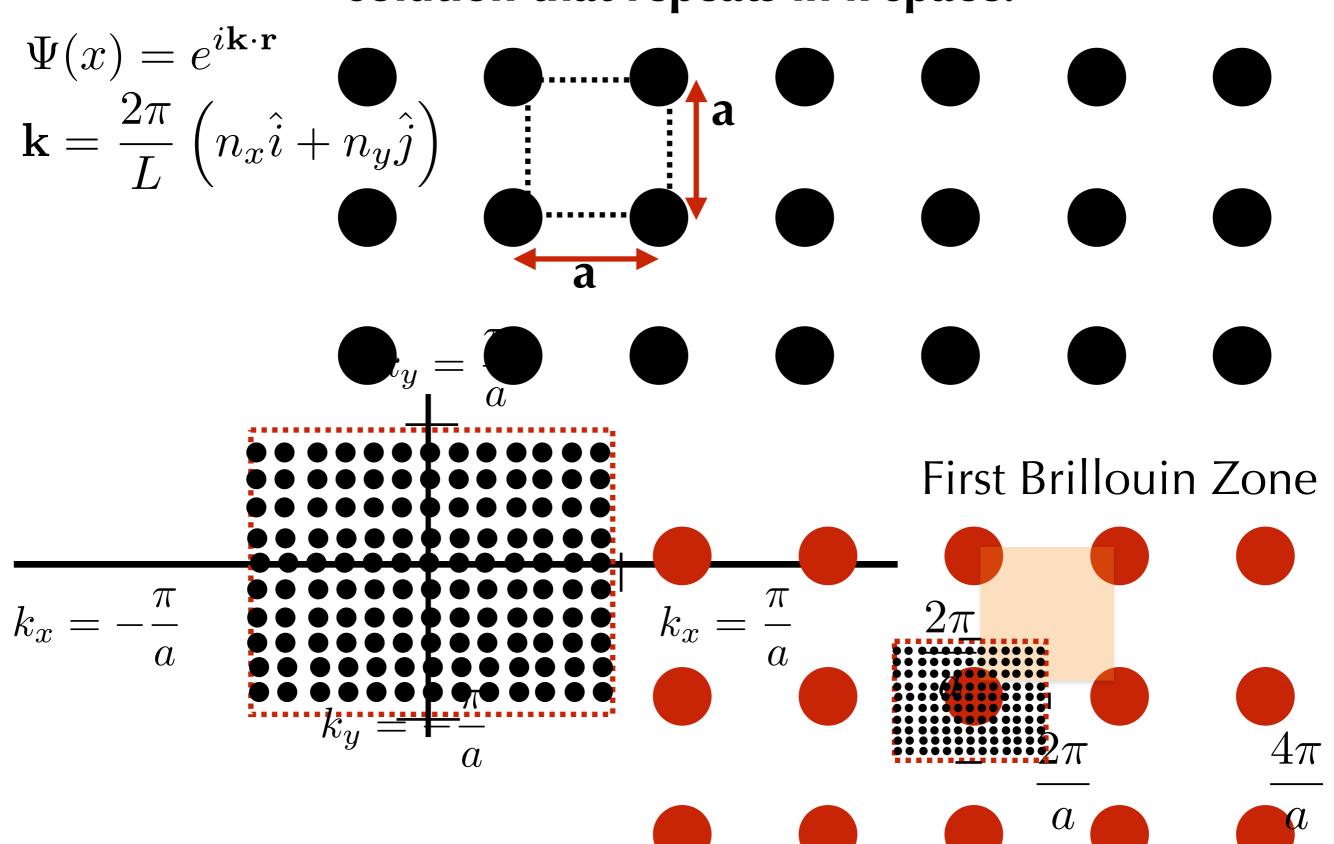
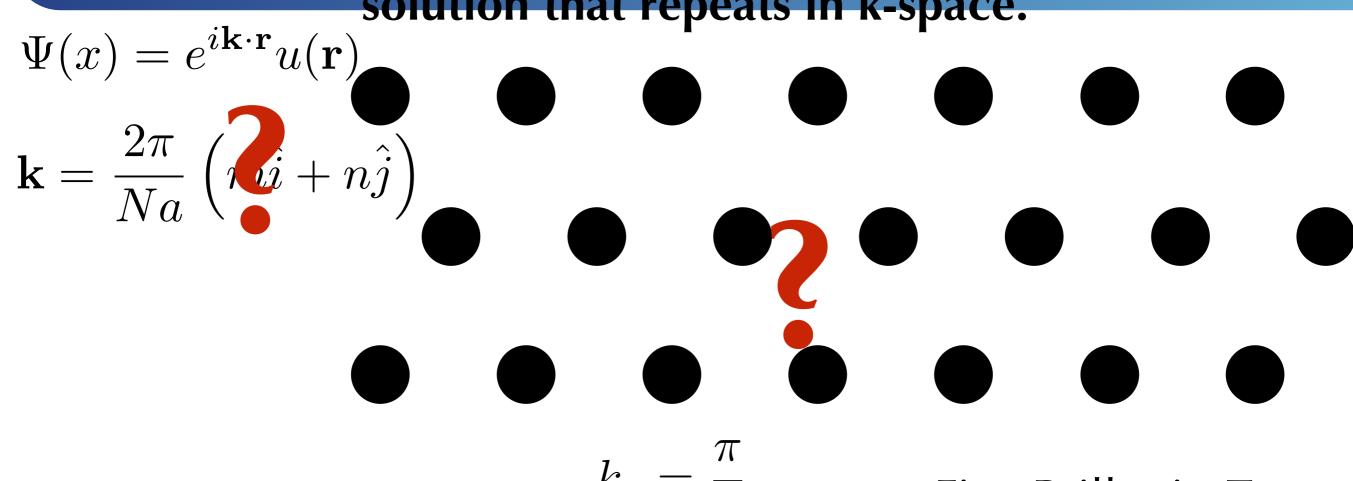


$$\frac{-2\pi}{a} \qquad 0 \qquad \frac{2\pi}{a} \qquad \frac{4\pi}{a} \qquad \frac{6\pi}{a}$$

A repeating atomic configuration in real space leads to a solution that repeats in k-space.



A repeating atomic configuration in real space leads to a solution that repeats in k-space.



$$k_y = \frac{\pi}{a}$$

First Brillouin Zone

$$k_x = -\frac{\pi}{a}$$

$$k_y = -$$

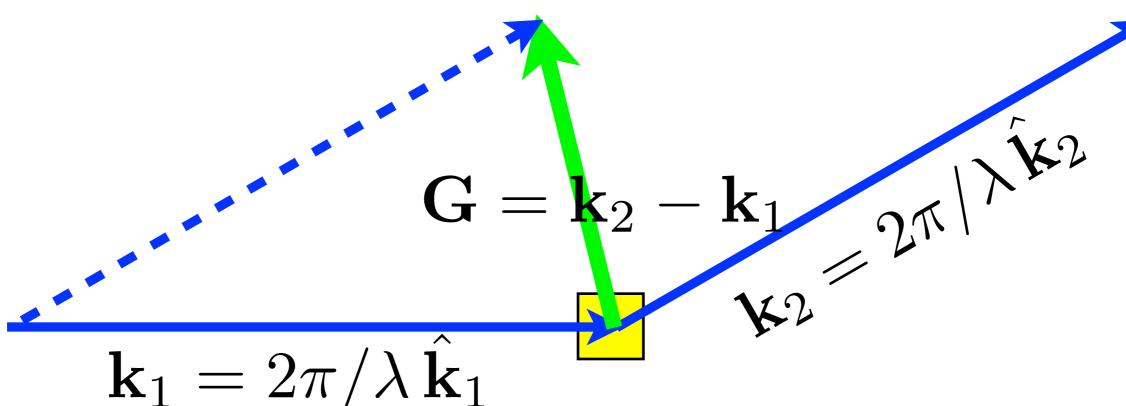
$$k_x = \frac{\pi}{a}$$

$$R\cos\theta_1 + R\cos\theta_2 = n\lambda$$

$$kR\cos\theta_1 + kR\cos\theta_2 = nk\lambda$$

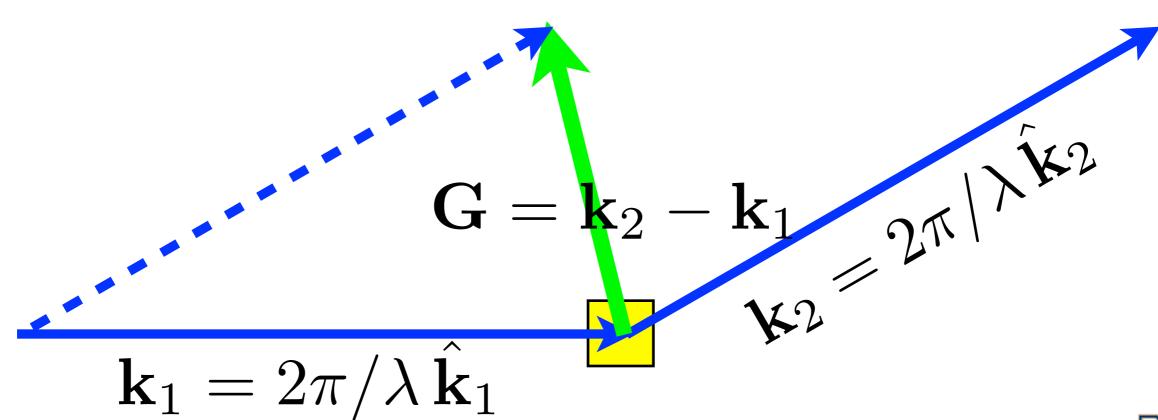
$$-\mathbf{R} \cdot \mathbf{k}_1 \qquad \mathbf{R} \cdot \mathbf{k}_2$$

$$\mathbf{R} \cdot \mathbf{G} = 2\pi n$$





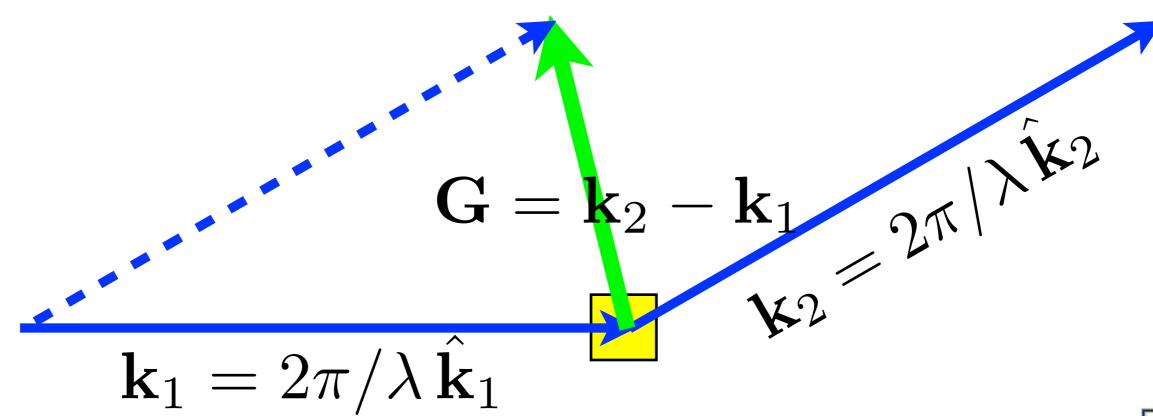
$$\mathbf{R} \cdot \mathbf{G} = 2\pi n$$





$$\mathbf{R} \cdot \mathbf{G} = 2\pi n$$

$$\mathbf{R} = m_1 \mathbf{a}_1 + m_2 \mathbf{a}_2 + m_3 \mathbf{a}_3$$





$$\mathbf{R} \cdot \mathbf{G} = 2\pi n$$

$$\mathbf{R} = m_1 \mathbf{a}_1 + m_2 \mathbf{a}_2 + m_3 \mathbf{a}_3$$

$$\mathbf{G} = n_1 \mathbf{b}_1 + n_2 \mathbf{b}_2 + n_3 \mathbf{b}_3$$



$$\mathbf{R} \cdot \mathbf{G} = 2\pi n$$

$$\mathbf{R} = m_1 \mathbf{a}_1 + m_2 \mathbf{a}_2 + m_3 \mathbf{a}_3$$

$$\mathbf{G} = n_1 \mathbf{b}_1 + n_2 \mathbf{b}_2 + n_3 \mathbf{b}_3$$

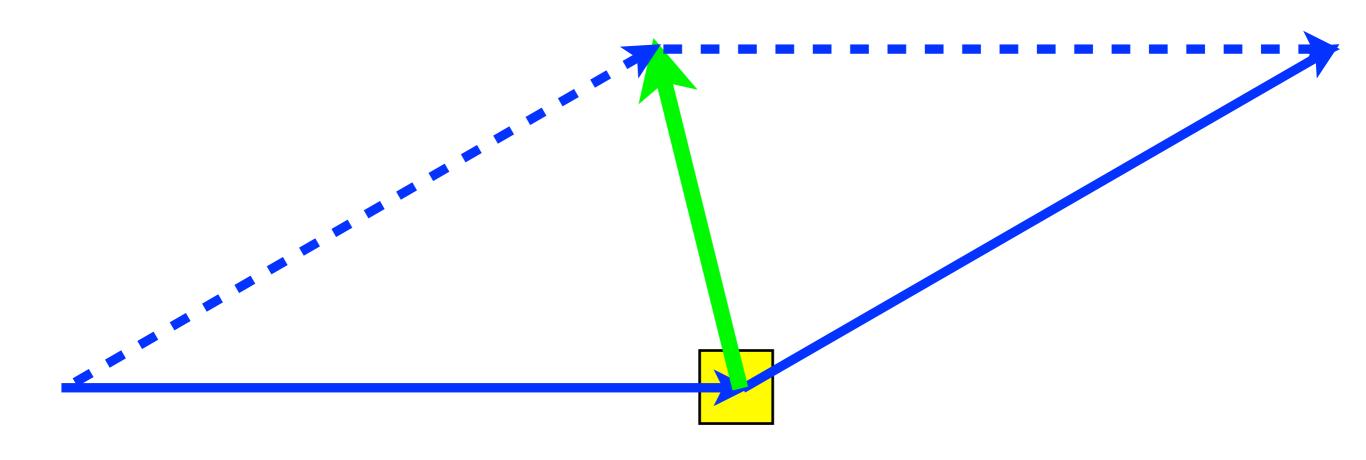
$$\mathbf{b}_i = 2\pi \frac{(\mathbf{a}_j \times \mathbf{a}_k)}{\mathbf{a}_i \cdot (\mathbf{a}_j \times \mathbf{a}_k)}$$



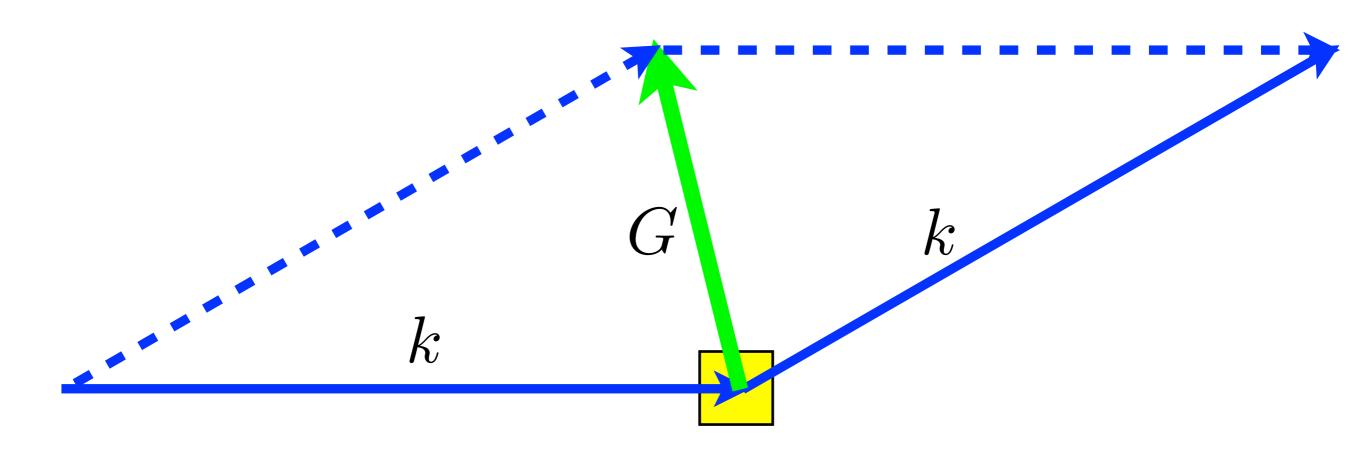
What is all this good for?



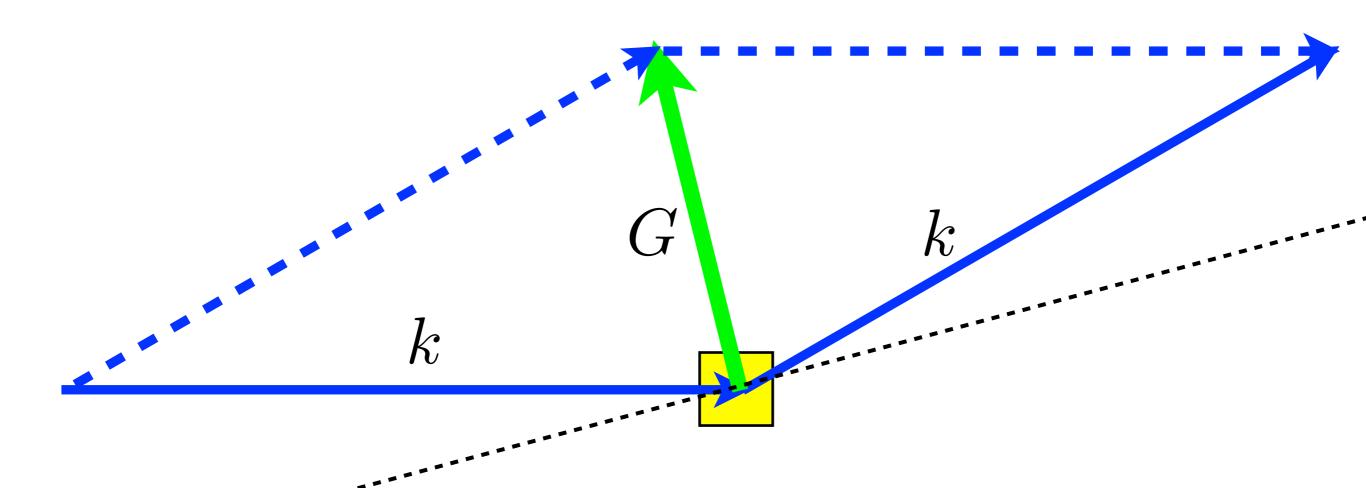




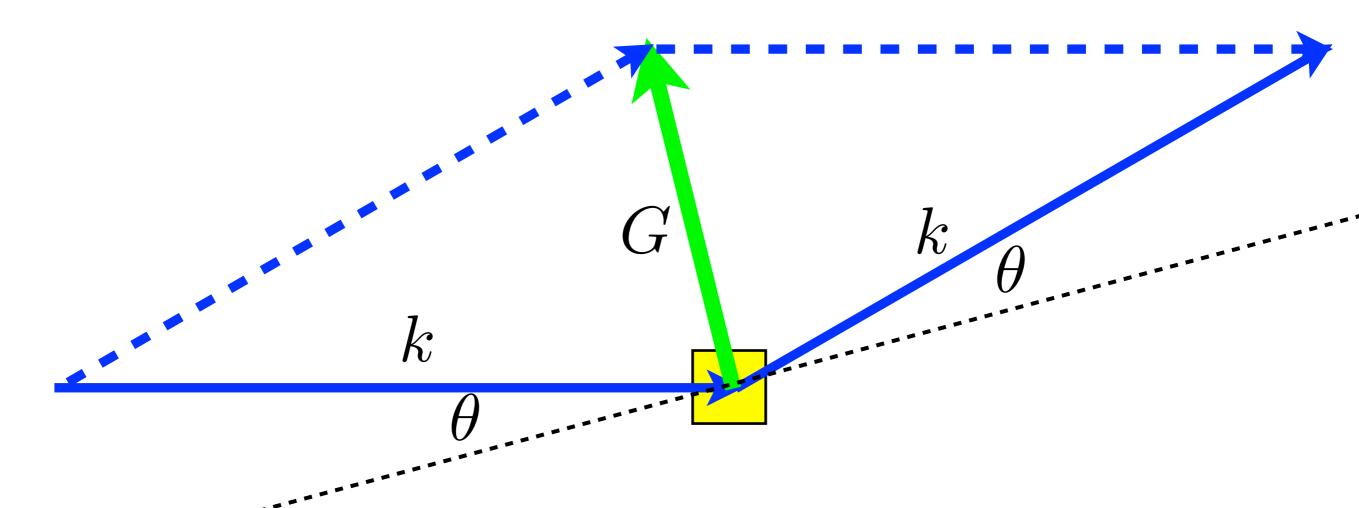




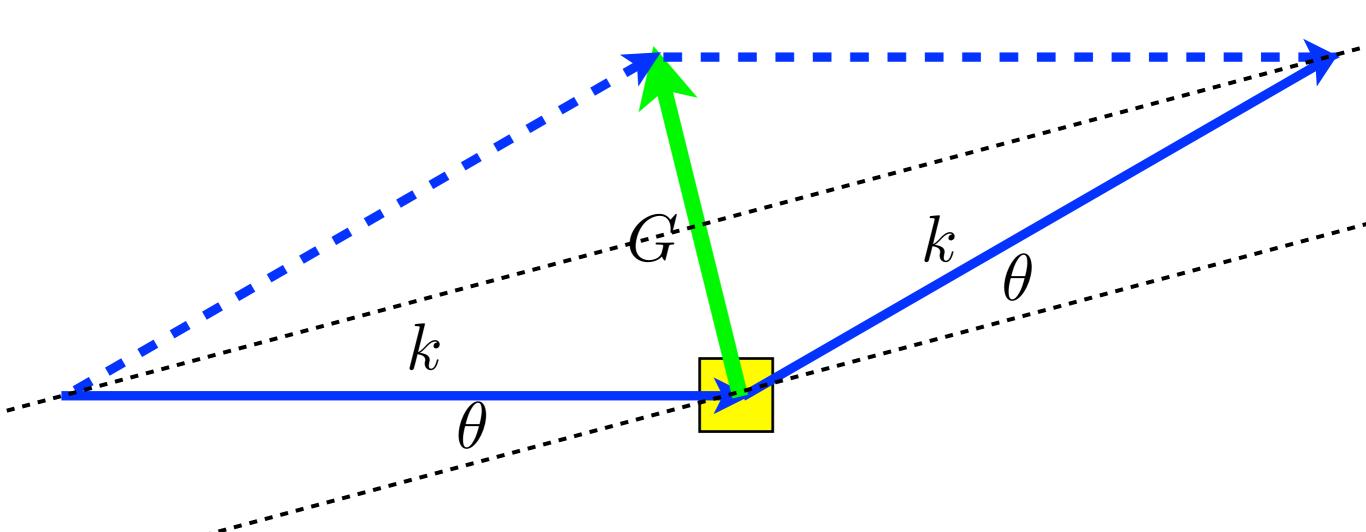




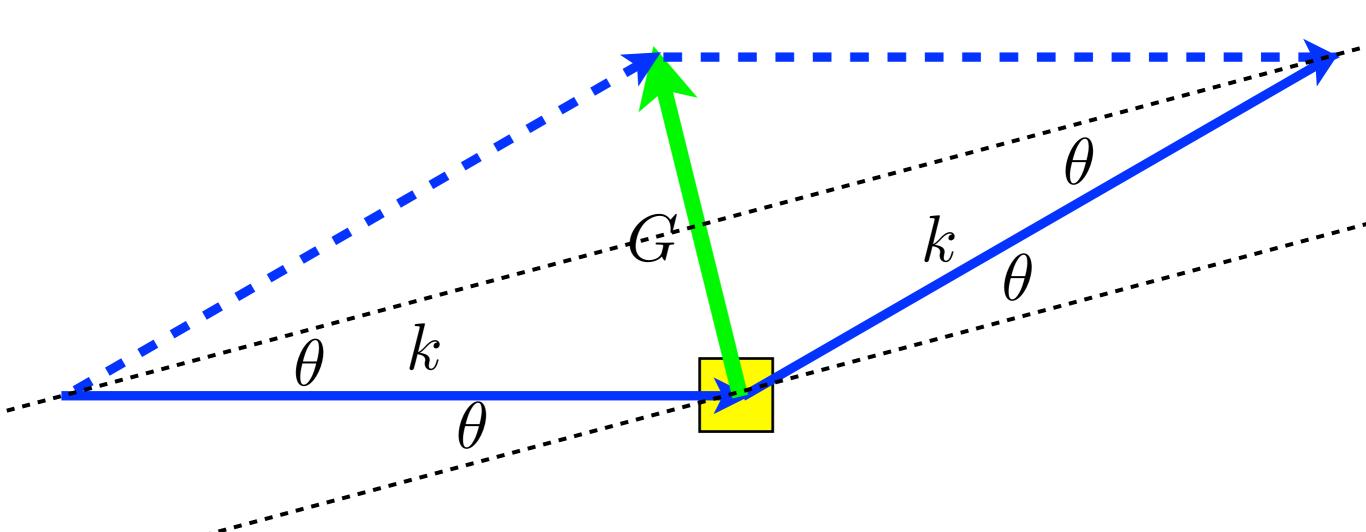




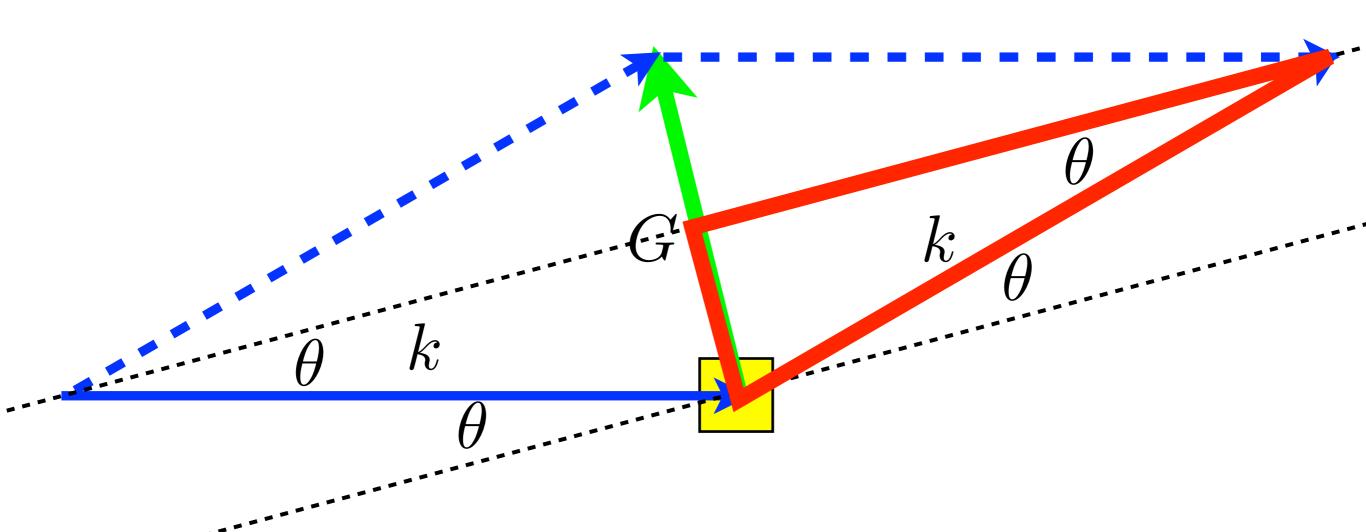




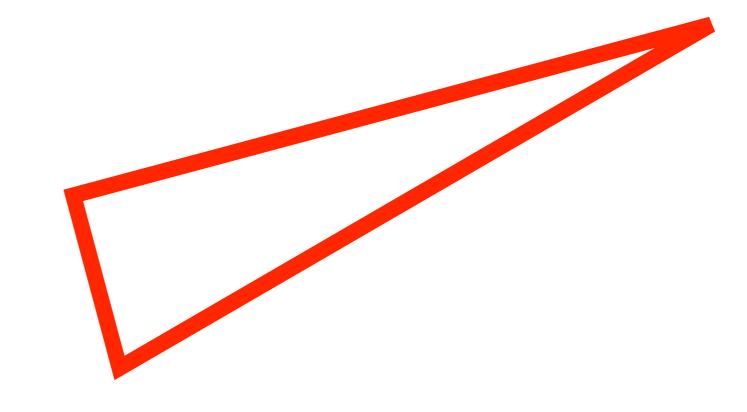














 θ k

 $\frac{G}{2}$



$$\frac{G}{2k} = \sin \theta$$

$$\frac{G}{2}$$

k



$$\frac{G}{2k} = \sin \theta$$

$$G \leq 2k$$



$$\frac{G}{2}$$



$$\mathbf{G} = n_1 \mathbf{b}_1 + n_2 \mathbf{b}_2 + n_3 \mathbf{b}_3$$

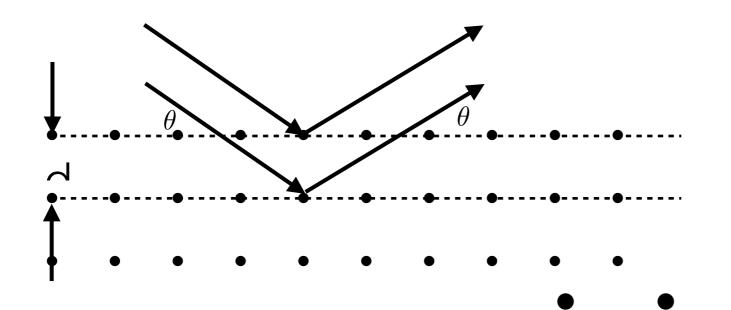
$$\frac{G}{2k} = \sin \theta$$

$$G \leq 2k$$



$$\frac{G}{2}$$





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

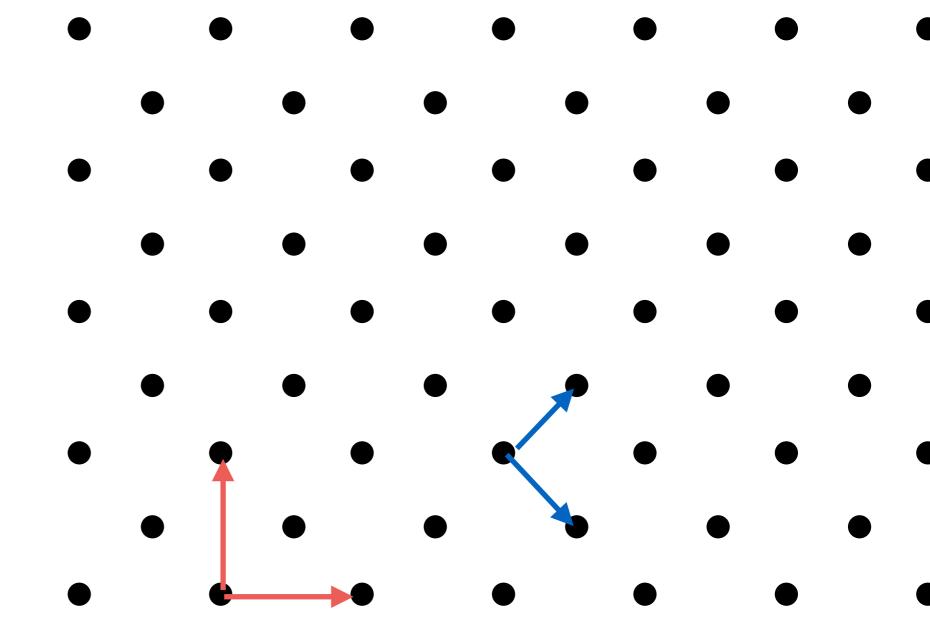
 $G = 2k\sin\theta$

• • • • •

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

$$\lambda = 1.542 \text{ Å}$$

$$a = 3.61 \text{ Å}$$



$$\mathbf{b}_{1} = 2\pi \frac{\mathbf{a}_{2} \times \mathbf{a}_{3}}{\mathbf{a}_{1} \cdot (\mathbf{a}_{2} \times \mathbf{a}_{3})}$$

$$\mathbf{b}_{2} = 2\pi \frac{\mathbf{a}_{3} \times \mathbf{a}_{1}}{\mathbf{a}_{2} \cdot (\mathbf{a}_{3} \times \mathbf{a}_{1})}$$

$$\mathbf{b}_{3} = 2\pi \frac{\mathbf{a}_{1} \times \mathbf{a}_{2}}{\mathbf{a}_{3} \cdot (\mathbf{a}_{1} \times \mathbf{a}_{2})}$$

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

$$\lambda = 1.542 \text{ Å}$$

$$a = 3.61 \text{ Å}$$

| h | | • | • | |
|---|--|---|---|---|
| 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 |
| $\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2)}$ $\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_3 \times \mathbf{a}_2}{\mathbf{a}_2 \cdot (\mathbf{a}_3)}$ | $ullet$ \mathbf{a}_3 \mathbf{a}_3 \mathbf{a}_3 | 90 46.6866 1 | 90 55.6621 | 90 64.7129 1 |

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

$$\mathcal{E} \propto f_e(\theta) \left[\sum_{\mathbf{R}} e^{i\mathbf{R} \cdot \Delta \mathbf{k}} \right] \sum_{\mathbf{r}_p} f_{ap}(\theta) e^{i\mathbf{r}_p \cdot \Delta \mathbf{k}} \qquad \lambda = 1.542 \; \mathring{\mathbf{A}} \\ a = 3.61 \; \mathring{\mathbf{A}} \\ 0. \qquad 12.3318 \qquad 25.2866 \qquad 39.8455 \qquad 58.6818 \\ \hline 17.5801 \qquad 25.2866 \qquad 28.5265 \qquad 37.1624 \qquad 59.3584 \qquad 72.7711 \\ \hline 39.8455 \qquad 42.4835 \qquad 59.3584 \qquad 64.9739 \qquad 90. - 20.9914 \; \mathbf{i} \\ 58.6818 \qquad 17.5801 \qquad 37.1624 \qquad 64.9739 \qquad 90. - 36.3554 \; \mathbf{i} \\ 17.5801 \qquad 25.2866 \qquad 42.4835 \qquad 72.7711 \qquad 90. - 20.9914 \; \mathbf{i} \\ 90. \qquad 37.1624 \qquad 42.4835 \qquad 58.6818 \qquad 90. - 23.9993 \; \mathbf{i} \qquad 90. - 46.6866 \; \mathbf{i} \\ 64.9739 \qquad 72.7711 \qquad 90. - 23.9993 \; \mathbf{i} \qquad 90. - 42.0372 \; \mathbf{i} \qquad 90. - 55.662 \; \mathbf{i} \\ 90. - 36.3554 \; \mathbf{i} \qquad 90. - 39.3563 \; \mathbf{i} \qquad 90. - 46.6866 \; \mathbf{i} \qquad 90. - 55.662 \; \mathbf{i} \qquad 90. - 64.7129 \; \mathbf{i} \\ \mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \\ \mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)} \\ \mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)}$$

$$\mathcal{E} \propto f_e(\theta) \left[\sum_{\mathbf{R}} e^{i\mathbf{R} \cdot \Delta \mathbf{k}} \right] \underbrace{\sum_{\mathbf{r}_p} f_{ap}(\theta) e^{i\mathbf{r}_p \cdot \Delta \mathbf{k}}}_{\mathbf{a} = 3.61 \text{ Å}} \lambda = 1.542 \text{ Å}$$

$$a = 3.61 \text{ Å}$$

$$0. \frac{12.3318}{25.2866} \frac{25.2866}{28.5265} \frac{28.5265}{37.1624} \frac{42.4835}{59.3584} \frac{58.6818}{61.7131} \frac{61.7131}{72.7711} \frac{72.7711}{90. -20.9914 \text{ i}} \frac{90. -20.9914 \text{ i}}{90. -36.3554 \text{ i}}$$

$$17.5801 \frac{37.1624}{17.5801} \frac{42.4835}{27.7711} \frac{58.6818}{90. -23.9993 \text{ i}} \frac{90. -36.3554 \text{ i}}{90. -36.3554 \text{ i}}$$

$$17.5801 \frac{25.2866}{42.4835} \frac{42.4835}{58.6818} \frac{90. -23.9993 \text{ i}}{90. -46.6866 \text{ i}} \frac{90. -36.3554 \text{ i}}{90. -36.3554 \text{ i}} \frac{90. -36.3554 \text{ i}}{90. -36.3554 \text{ i}}$$

$$17.5801 \frac{37.1624}{90. -36.3554 \text{ i}} \frac{42.4835}{90. -23.9993 \text{ i}} \frac{90. -46.6866 \text{ i}}{90. -55.662 \text{ i}} \frac{90. -64.7129 \text{ i}}{90. -64.7129 \text{ i}}$$

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

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

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

```
\lambda = 1.542 \text{ Å}
                                                                a = 3.61 \text{ Å}
  h
                                          20 2455
                   12 2218
                              25.2866
                                                            58.6818
                   17.5801
                                          42.4835
                              37.1624
                                                            72.7711
       25.2866
                                                            90. - 20.9914 i
                                          64.9739
                   42.4835
                                          90. - 20.9914 i
                                                            90. - 36.3554 i
       58.6818
                              72.7711
h
                  17.5801
                                                                    90. - 36.3554 i
  Θ.
                                   37.1624
                                                   64.9739
  17.5801
                  25,2866
                                                   72.7711
                                                                    90. - 39.3563 i
                                   42.4835
  37.1624
                                                   90. - 23.9993 i 90. - 46.6866 i
                  42.4835
                                   58.6818
  64.9739
                                   90. – 23.9993 i
                                                   90. - 42.0372 i 90. - 55.662 i
                  72.7711
  90. - 36.3554 i
                  90. - 39.3563 i 90. - 46.6866 i
                                                   90. – 55.662 i
                                                                    90. - 64.7129 i
       Θ.
                             25.2866
                                           58.6818
                                                         90. - 42.0372 i
       17.5801
                             17.5801
                                           42.4835
                                                         90. – 23.9993 i
       37.1624
                             25.2866
                                           37.1624
                                                         72.7711
       64.9739
                             42.4835
                                           42.4835
                                                         64.9739
       90. – 36.3554 i
                             72.7711
                                           58.6818
                                                         72.7711
```

$$\mathcal{E} \propto f_e(\theta) \left[\sum_{\mathbf{R}} e^{i\mathbf{R} \cdot \Delta \mathbf{k}} \right] \underbrace{\sum_{\mathbf{r}_p} f_{ap}(\theta) e^{i\mathbf{r}_p \cdot \Delta \mathbf{k}}}_{\mathbf{a} = 3.61 \text{ Å}} \lambda = 1.542 \text{ Å}$$

$$a = 3.61 \text{ Å}$$

$$b_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$b_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)}$$

$$b_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)}$$

$$\mathcal{E} \propto f_e(\theta) \left[\sum_{\mathbf{R}} e^{i\mathbf{R} \cdot \Delta \mathbf{k}} \right] \sum_{\mathbf{r}_p} f_{ap}(\theta) e^{i\mathbf{r}_p \cdot \Delta \mathbf{k}} \qquad \lambda = 1.542 \text{ Å}$$

$$a = 3.61 \text{ Å}$$

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

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

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

$$\mathcal{E} \propto f_e(\theta) \left[\sum_{\mathbf{R}} e^{i\mathbf{R} \cdot \Delta \mathbf{k}} \right] \left[\sum_{\mathbf{r}_p} f_{ap}(\theta) e^{i\mathbf{r}_p \cdot \Delta \mathbf{k}} \right] \quad \begin{array}{c} \lambda = 1.542 \text{ Å} \\ a = 3.61 \text{ Å} \end{array}$$

| 0. | 8.20862 | 16.5921 | 25.3618 | 34.8277 |
|---------|---------|---------|---------|-----------------|
| 12.3318 | 14.8864 | 20.8909 | 28.5957 | 37.5706 |
| 25.2866 | 26.7679 | 30.9177 | 37.2228 | 45.494 |
| 39.8455 | 41.0286 | 44.5453 | 50.4176 | 59.127 |
| 58.6818 | 60.0134 | 64.2575 | 72.8742 | 90. – 13.4335 i |

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

$$\mathcal{E} \propto f_e(\theta) \left[\sum_{\mathbf{R}} e^{i\mathbf{R} \cdot \Delta \mathbf{k}} \right] \left[\sum_{\mathbf{r}_p} f_{ap}(\theta) e^{i\mathbf{r}_p \cdot \Delta \mathbf{k}} \right] \quad \lambda = 1.542 \text{ Å}$$

$$a = 3.61 \text{ Å}$$

| Θ. | 16.5921 | 34.8277 | 58.9444 | 90. – 30.2067 i |
|---------|-----------------|---------|---------|-----------------|
| 14.8864 | 14.8864 | 28.5957 | 48.1721 | 90. – 11.999 i |
| 30.9177 | 25.2866 | 30.9177 | 45.494 | 73.1867 |
| 50.4176 | 41.0286 | 41.0286 | 50.4176 | 73.5869 |
| 90 13 | .4335 i 64.2575 | 58.6818 | 64.2575 | 90. – 13.4335 i |

| Θ. | 8.20862 | 16.5921 | 25.361 8 | 34.8277 |
|--|--------------------------------------|--------------------|---------------------|---------------------|
| 12.331 8 | 14.8864 | 20.8909 | 28.5957 | 37.570 6 |
| 25.2866 | 26.7679 | 30.9177 | 37.2228 | 45.494 |
| 39.845 5 | 41.0286 | 44.5453 | 50.4176 | 59.127 |
| 58.6818 | 60.0134 | 64.2575 | 72.874 2 | 90. – 13.4335 i |
| $\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \wedge \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)} \bullet \bullet \bullet \bullet$ | | | | |
| a 3 · | $(\mathbf{a}_1 \wedge \mathbf{a}_2)$ | | | |