## **Overview of Phase Contrast & High resolution TEM**

Lecture 14

Incident electron wave	
Sample (very thin!)	
Transmitted & Diffracted waves	

Transmitted & diffracted waves each have a different phase

Result is an interference pattern - our 'phase contrast' or HREM image





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Why are the phases different?

**Transmitted & diffracted waves are allowed** wave functions in the crystal

 Together they form the "Exit Wave" which leaves the crystal

They solve Schrödinger's Equation  $\nabla^{2}\psi\left(\stackrel{r}{\mathbf{r}}\right) + \frac{8\pi m e}{h^{2}}\left[E + V\left(\stackrel{r}{\mathbf{r}}\right)\right]\psi\left(\stackrel{r}{\mathbf{r}}\right) = 0$ Solutions are Bloch Waves:  $b^{(j)}\left(\stackrel{r}{\mathbf{k}}^{(j)}, \stackrel{r}{\mathbf{r}}\right) = \sum_{g} C_{g}^{(j)} \operatorname{gexp}\left[2\pi i\left(\stackrel{r}{\mathbf{k}}^{(j)} + \stackrel{r}{g}\right)\stackrel{r}{\mathbf{r}}\right]$ Amplitude term Phase term

### Looking at these Bloch waves:

$$\mathbf{b}^{(j)}\left(\vec{\mathbf{r}}\right) = \sum_{g} \mathbf{C}_{g}^{(j)} \operatorname{gexp}\left[2\pi i\left(\mathbf{k}^{(j)} + \mathbf{g}\right)\mathbf{r}\right]$$

Phase term has to do with the strength & spacing of the periodic potential of the lattice along a given direction in the crystal (g)

Different diffracted waves have different phase shifts

# The total "Exit Wave" is thus the sum over all of the Bloch waves

$$\psi_{\text{total}} = \sum_{j=1}^{n} \mathcal{A}^{(j)} \psi^{(j)} = \sum_{j=1}^{n} \mathcal{A}^{(j)} \mathbf{b} \left( \mathbf{k}^{(j)}, \mathbf{r} \right)$$



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- So, appears "simple" enough ...
- (1) Calculate the phase differences for the different diffracted waves
- (2) Create an interference pattern from the overlap of these phases in two-dimensions

#### Not even this "simple"

#### The TEM has very poor lenses

 Spherical aberration in particular

This aberration causes diffracted waves to be 'phase shifted' by the objective lens

- Complex dependence on wavelength,  $C_{s,}$  diffraction vector and defocus
- Magnitude of shift varies with distance from optic axis
  - And thus diffraction angle
  - Thus each diffracted wave undergoes a different phase shift

#### **Complicates image** interpretation



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**Returning to this picture** 

This means that the phases of the diffracted waves are changed by the objective lens focus

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Thus, the image you get STRONGLY DEPENDS ON THE FOCUS CONDITION

# A single HREM image

Image courtesy C. Kisielowski, NCEM, LBNL

#### The 'unscrambled' exit wave

Simulation: Si

0.18 nm