Friedrich-Alexander-Universität
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DISCUS Workshop
Modulated structures

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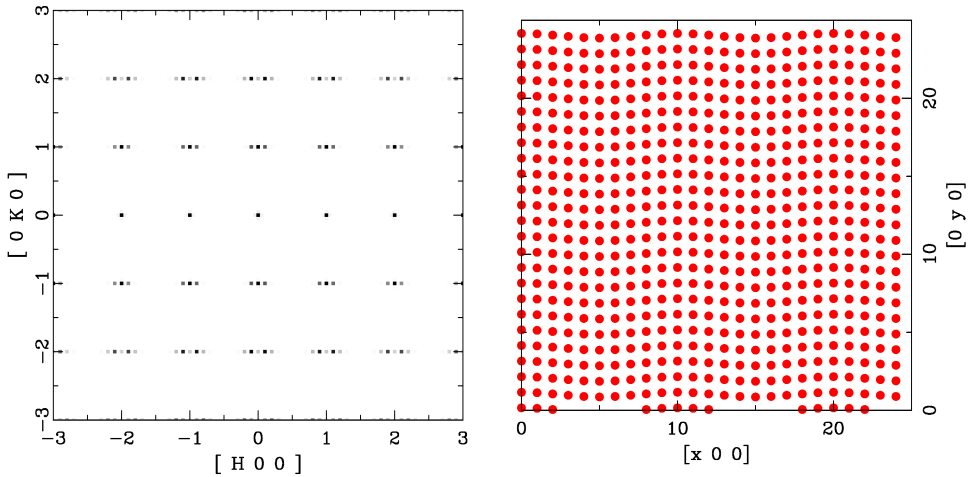
Modulated structures

A basic **average** structure with unit cell a,b, c, α, β, γ

An additional **moderate to long range**
ordering scheme
along one or two **direction**

wave length often or arbitrary length

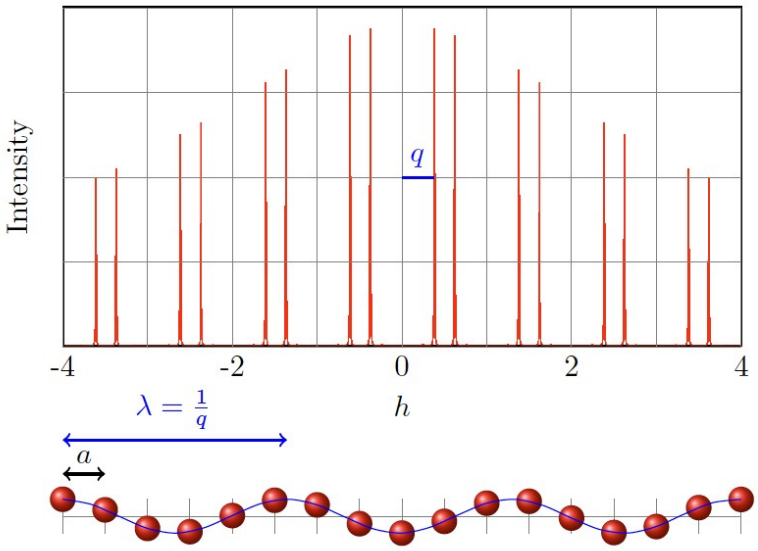


Additional satellite reflections

Modulated structures

Modulation function as **wave** throughout structure

Additional satellite reflections



Main Bragg reflections omitted

Bragg reflections: $h \in \mathbb{Z}$

Satellite reflections: $h \pm mq$ $h, m \in \mathbb{Z}$

$$\vec{u}(\vec{r}) = \vec{A}\cos\left(2\pi\left(\vec{q}\,\vec{r} + t\right)\right)$$

Transverse: $\vec{A} \perp \vec{r}$

Longitudinal: $\vec{A} \parallel \vec{r}$

$$\rho(\vec{r}) = \rho\cos\left(2\pi\left(\vec{q}\,\vec{r} + t\right)\right)$$

Density / Charge density / ...

Modulated structures

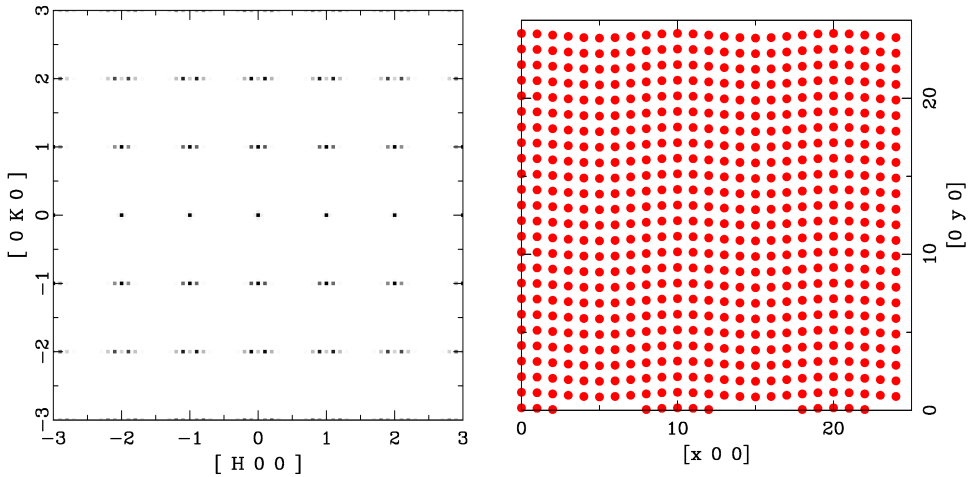
Reflection conditions for displacement waves

$$\vec{u}(\vec{r}) = \vec{A}\cos\left(2\pi\left(\vec{q}\,\vec{r} + t\right)\right)$$

In reciprocal space at regions where

$$\vec{r} \perp h\vec{k}l + \vec{q}$$

satellites have zero intensity



Calculating a powder diffraction pattern

Open in Windows Explorer: Lectures\12_Modulated\

Start DISCUS_SUITE

You should see:

...
User macros in ...
System macros in ...
Start directory ...

suite >

suite > **cd Lectures\12_Modulated**

suite > **@main.mac**

suite > **@density.mac**

Wave build a modulated structure

Main steps

Wave vector: **vector** Direct space components

Wavelength: **length** [Å]

Type: **trans**; **long**; **density**

Amplitude:

displacement **amplitude** [Å]

density **plow** and **phigh** plus **replace**

Phase at 0,0,0: **phase**

Wave function **sinus**; **box**; **triang**

Wave build a modulated structure

complete.mac

```
wave
reset      # Ensure clean start up conditions
vector      1.00, 0.00, 0.00  # Set wave vector as [ U, V, W ]
amplitude   lat[2]*0.15       # Set the amplitude in Angstroem
function    sinus             # Use sinusoidal function grid
lenght      lat[1]*10.0       # Set wave length in Angstroem
transverse                    # Select displacement style
accoustic                     # all atoms displaced in same direction
                              # ==> opticcal
phase      0.00               # Phase at coordinates 0,0,0
```