

# Sources and Optics for XAS



Apurva Mehta



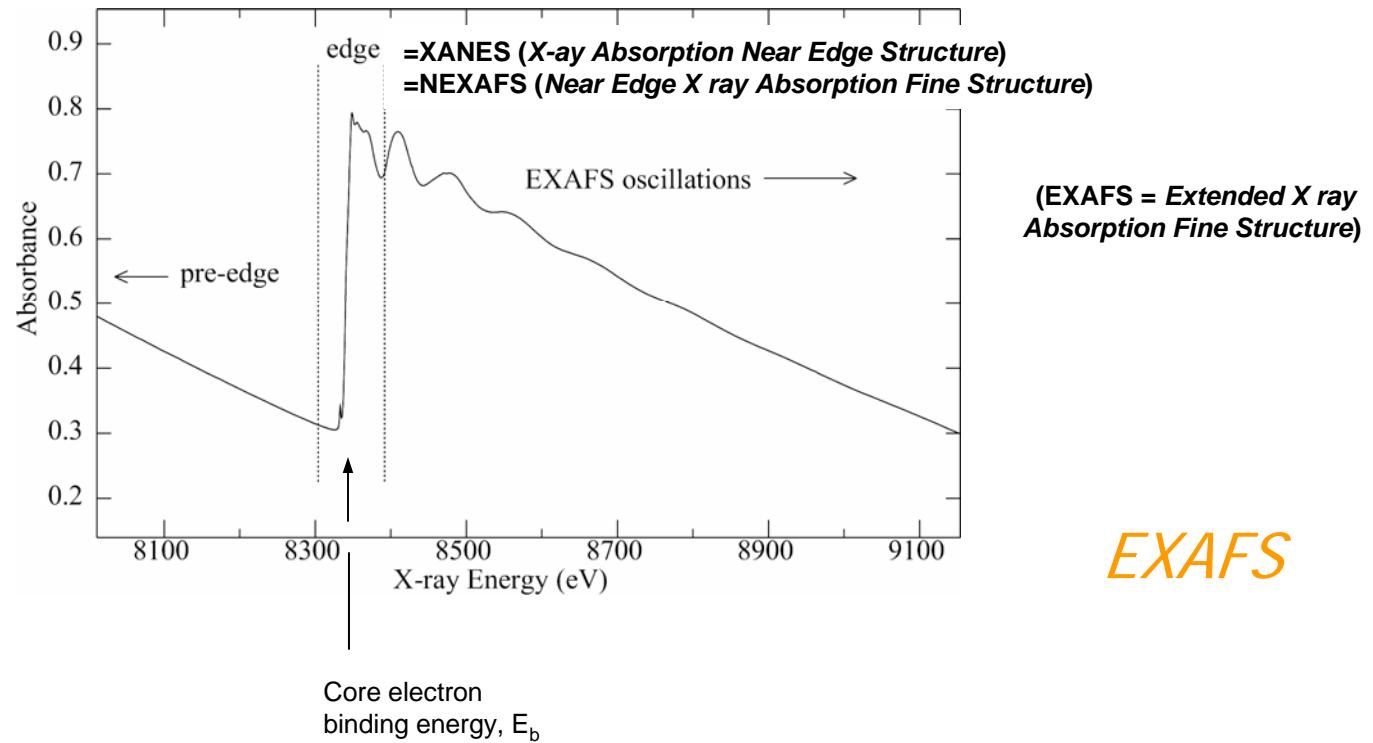
*Stanford Synchrotron Radiation  
Laboratory*

# *X-ray absorption Spectroscopy*

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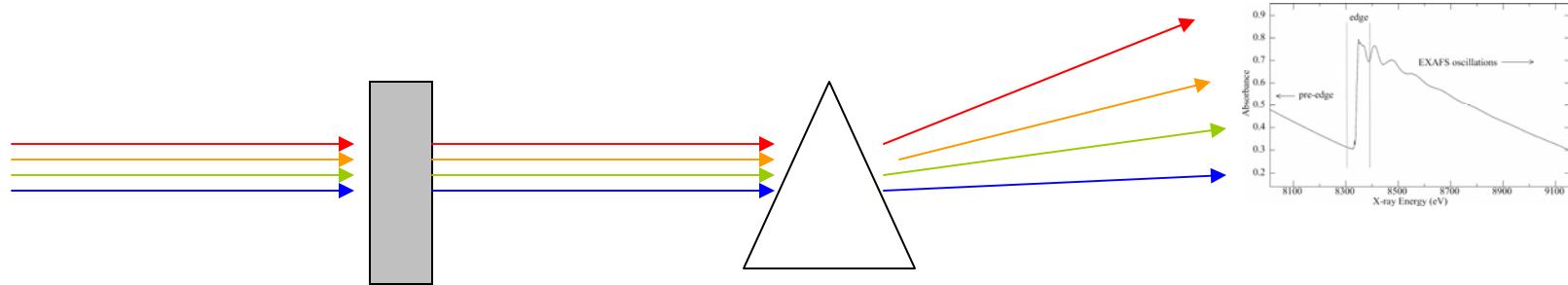


## ***Basic Experiment :***



# Two ways of collecting data

## *White Beam Energy Dispersive*



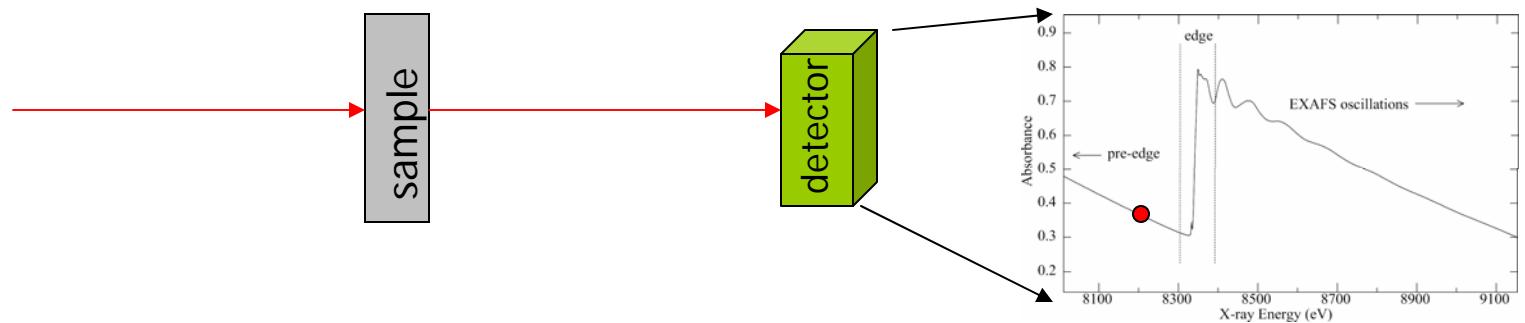
Spectrum in Single Shot

Optics and Detector are not Available

LCLS/fast changes

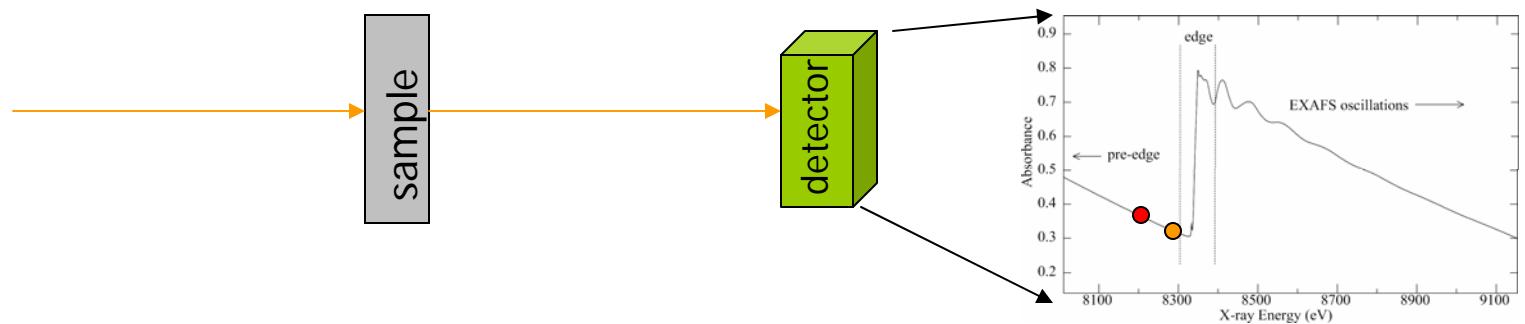
# Two ways of collecting data

## *Monochromatic "Scanning" Measurement*



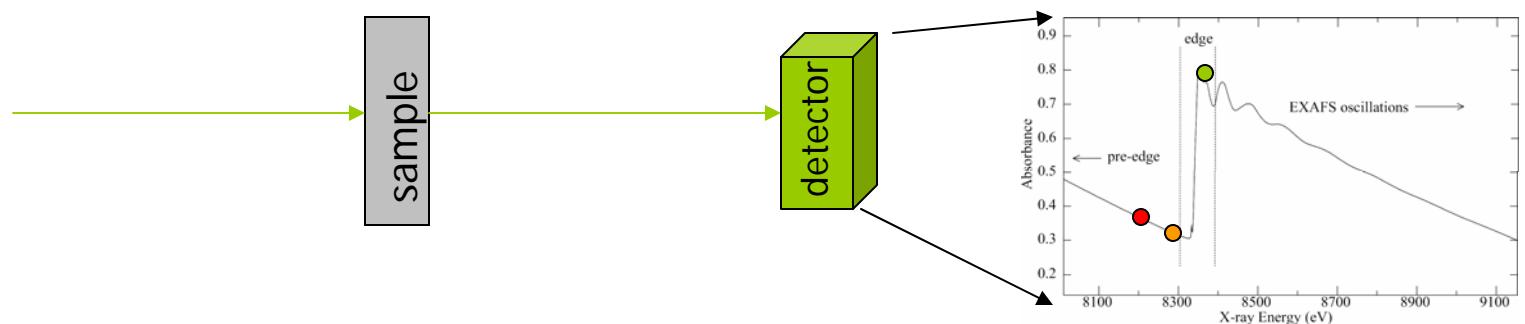
# Two ways of collecting data

## *Monochromatic "Scanning" Measurement*



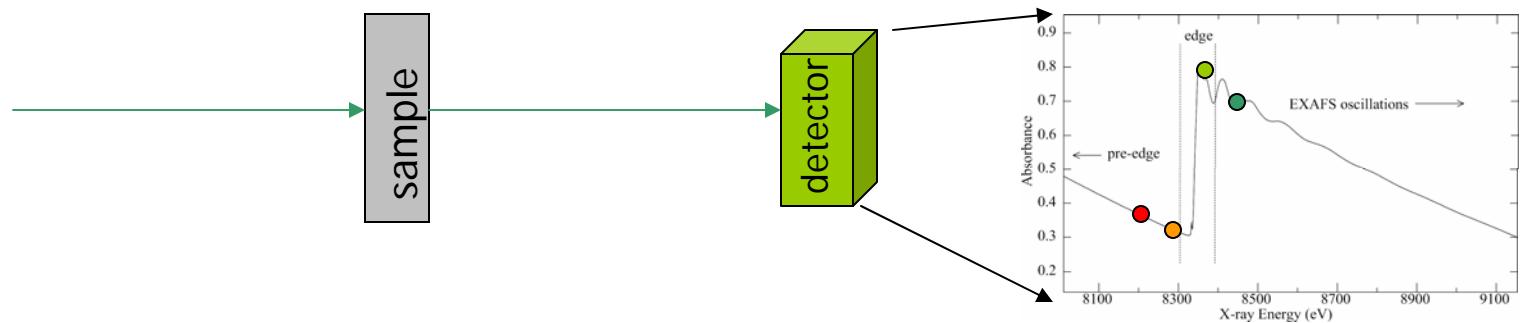
# Two ways of collecting data

## *Monochromatic "Scanning" Measurement*



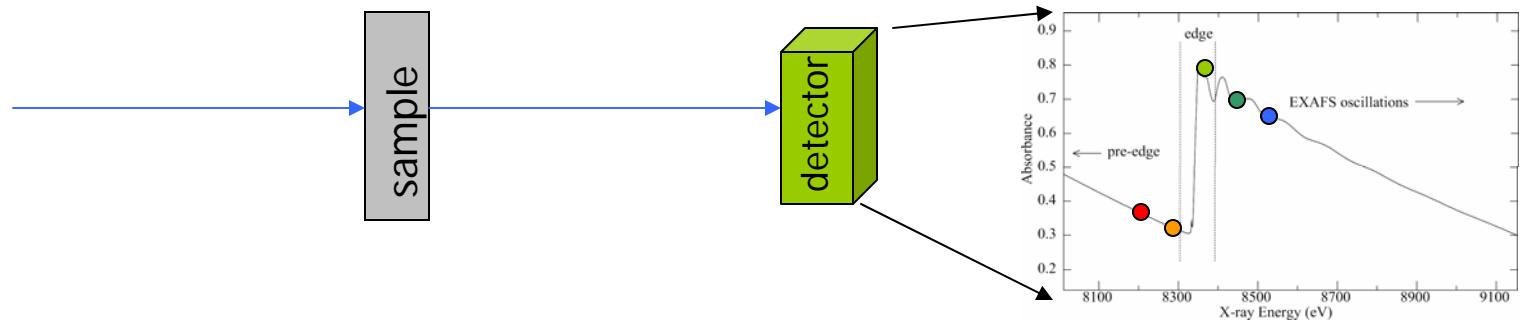
# Two ways of collecting data

## *Monochromatic "Scanning" Measurement*



# Two ways of collecting data

## *Monochromatic "Scanning" Measurement*



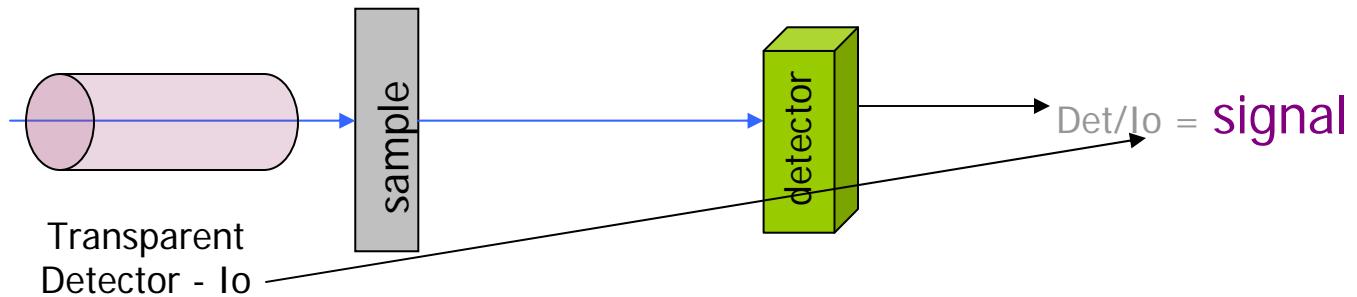
Slow but doable



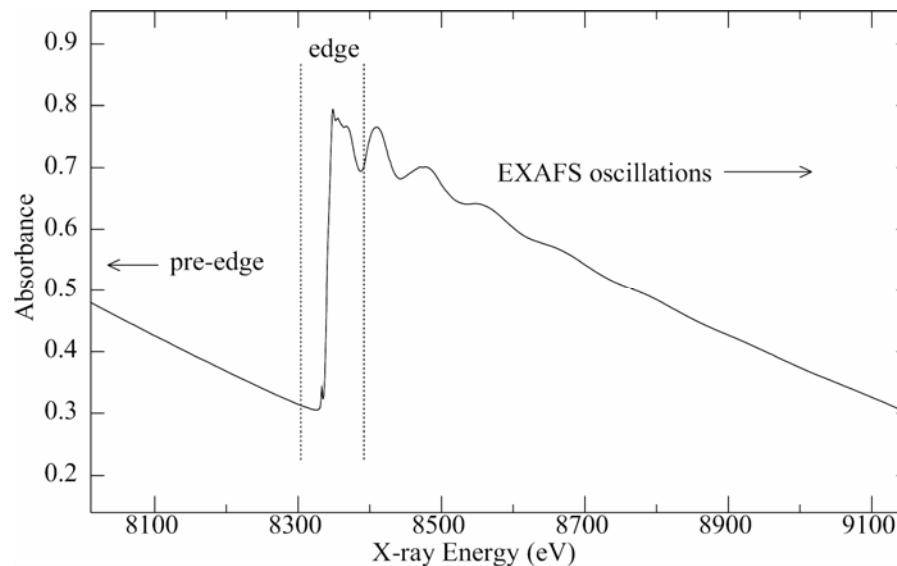
# Outline

- ◆ Sources
  - ◆ Wiggler vs. Undulator
- ◆ Slits
- ◆ Monochromator
  - ◆ Energy Resolution
  - ◆ “Glitches”
  - ◆ Harmonic rejection
- ◆ Mirrors
- ◆ High Flux Density
- ◆ XAS BL Layout

# Measurement Requirements

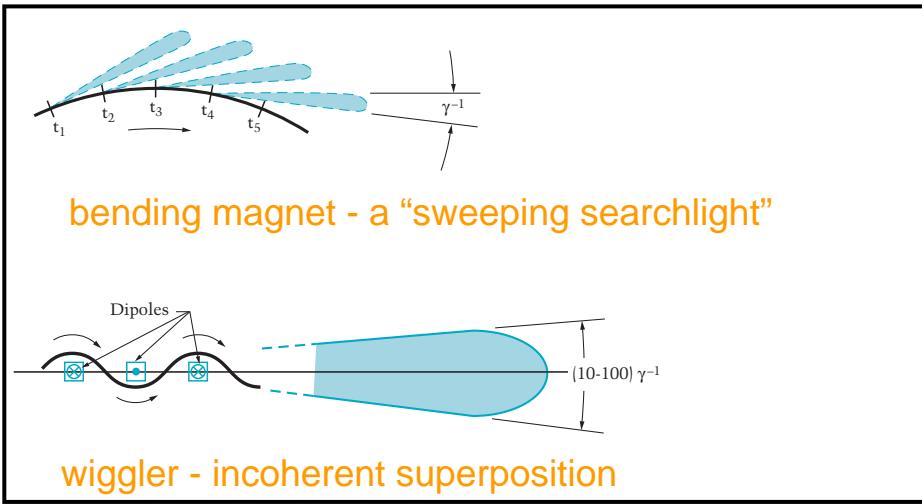
*Xanes**Energy Resolution**EXAFS*

*Very Robust*  
*Normalization*  
*Homogeneous Beam*

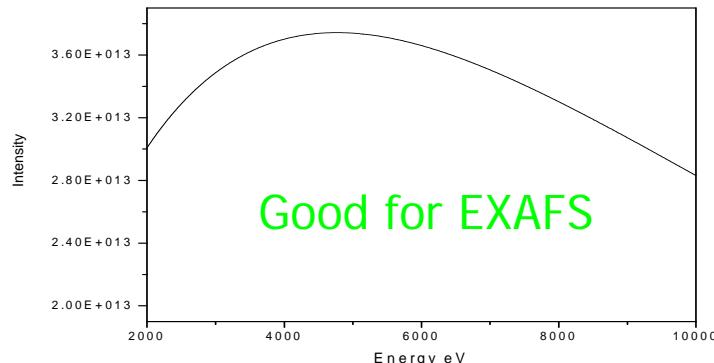
*Very High*  
*Signal to Noise*



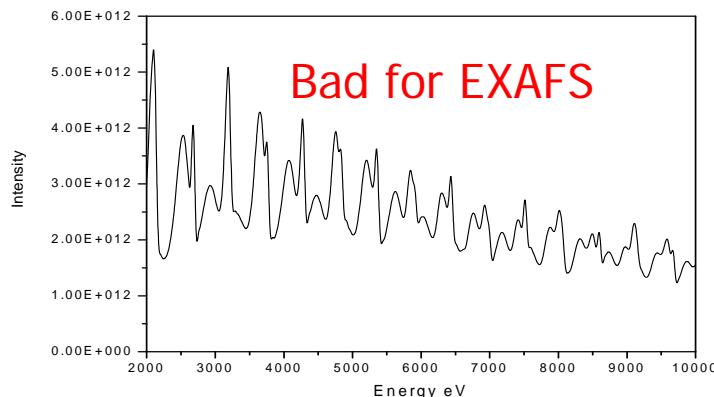
# Sources



## Bend magnets and Wigglers



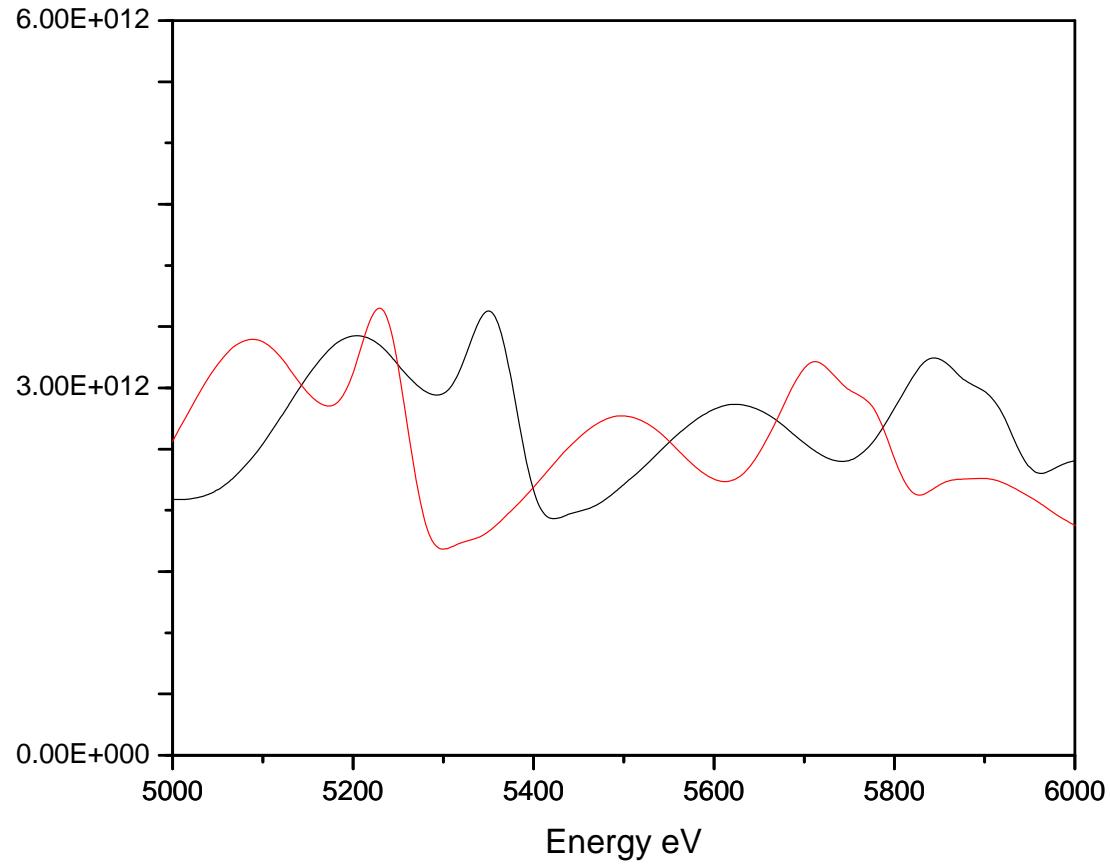
## Undulators



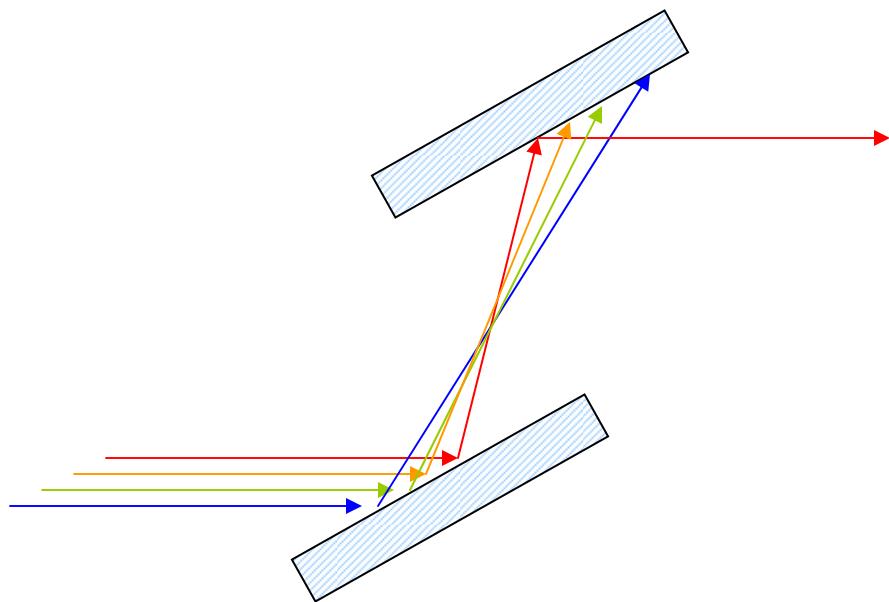


# How to Use an Undulator

*Changing the Undulator K – Scanning the Gap*



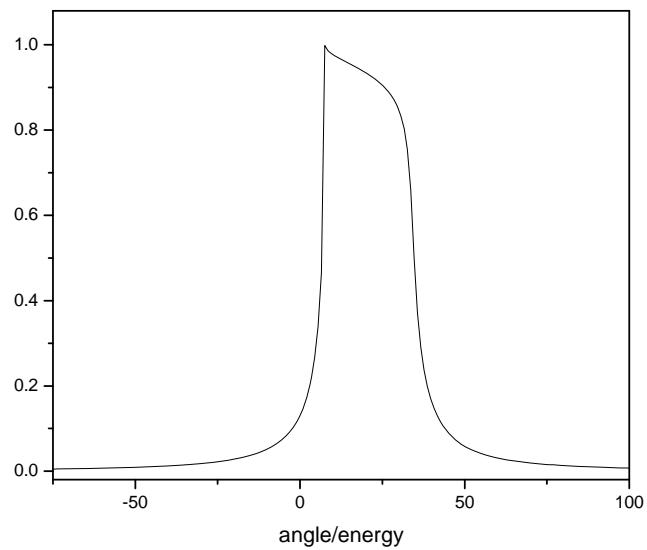
# Double Crystal Monochromator



Bragg's Law:

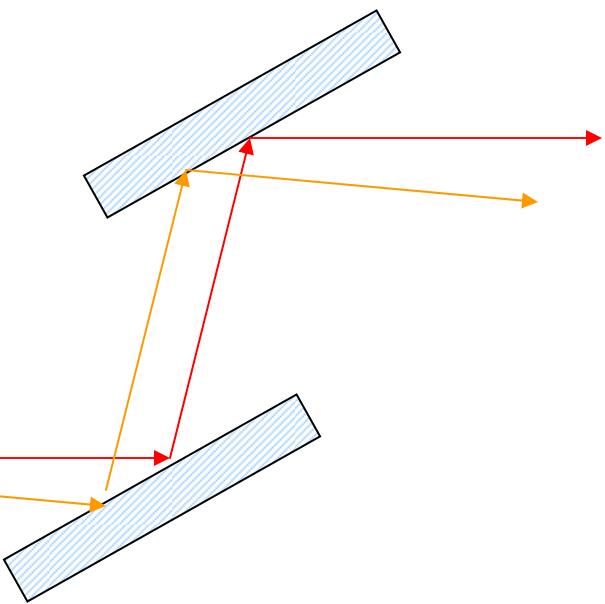
$$2d\sin(\theta) = h/E$$

*Not Right!*

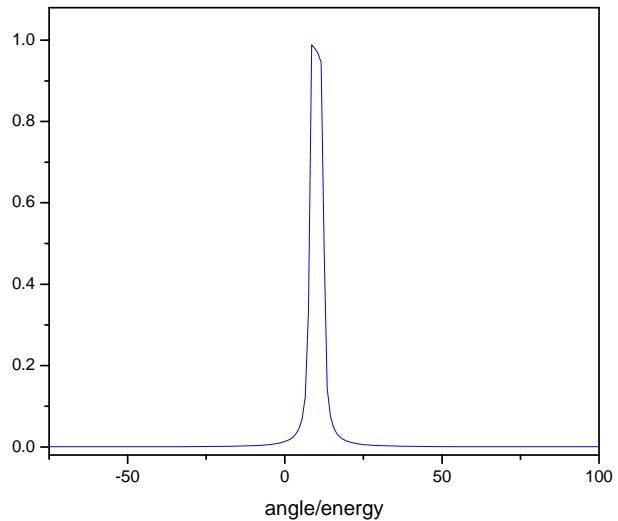
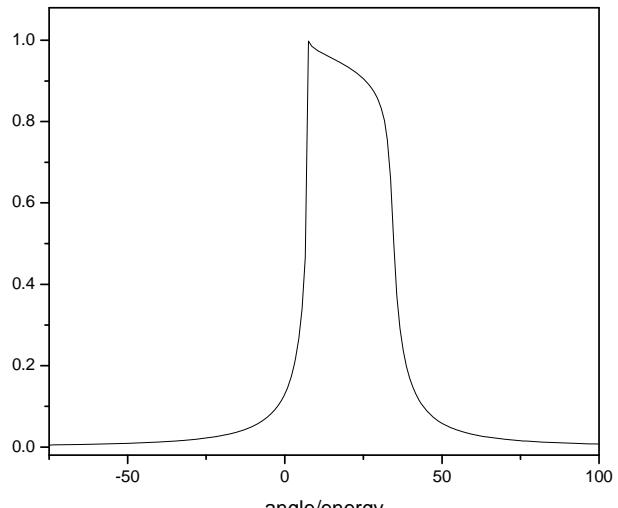


# Double Crystal Monochromator

## Increasing Energy Resolution

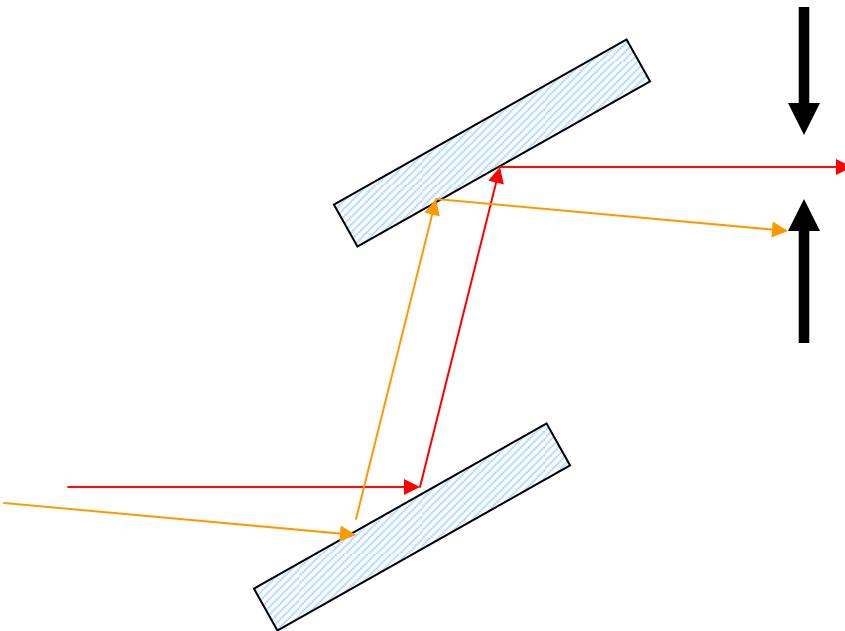


Use Higher Order Reflection



# Double Crystal Monochromator

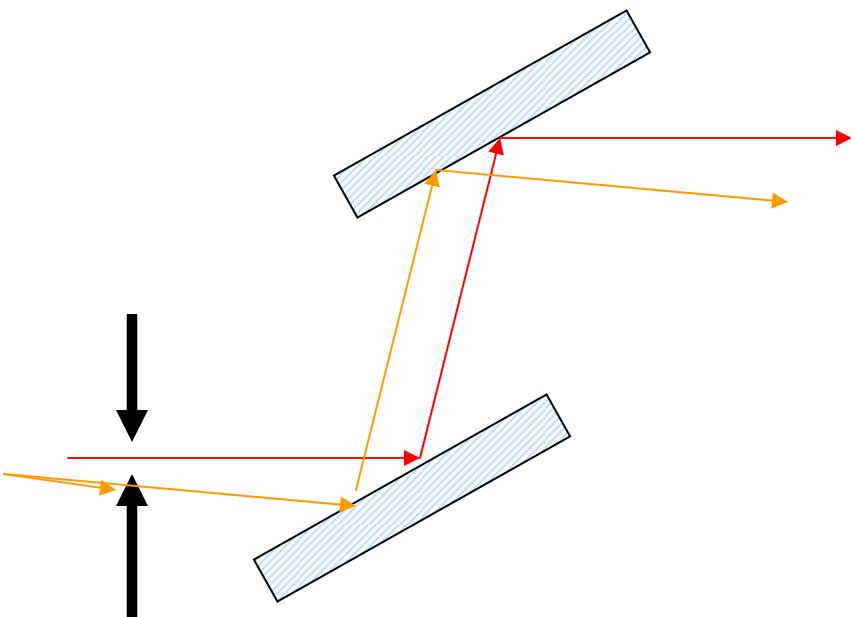
Increasing Energy Resolution



Use Narrower In Slits

# Double Crystal Monochromator

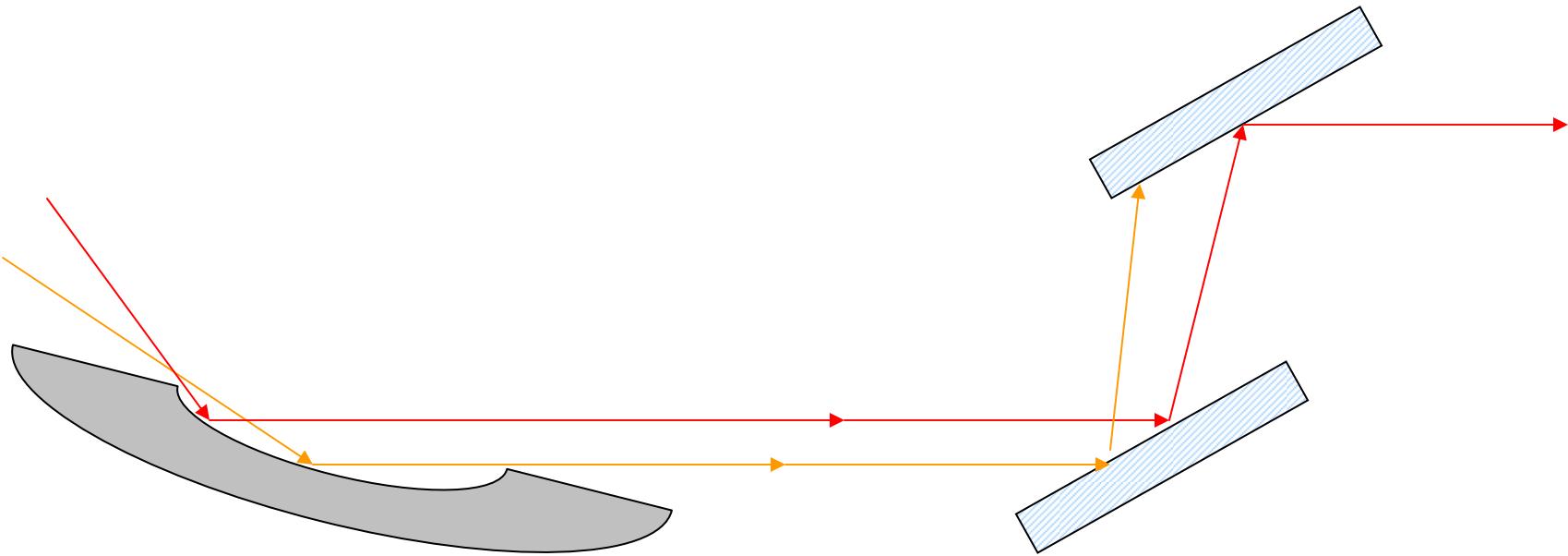
Increasing Energy Resolution



Use Narrower Mono  
Slits

# Double Crystal Monochromator

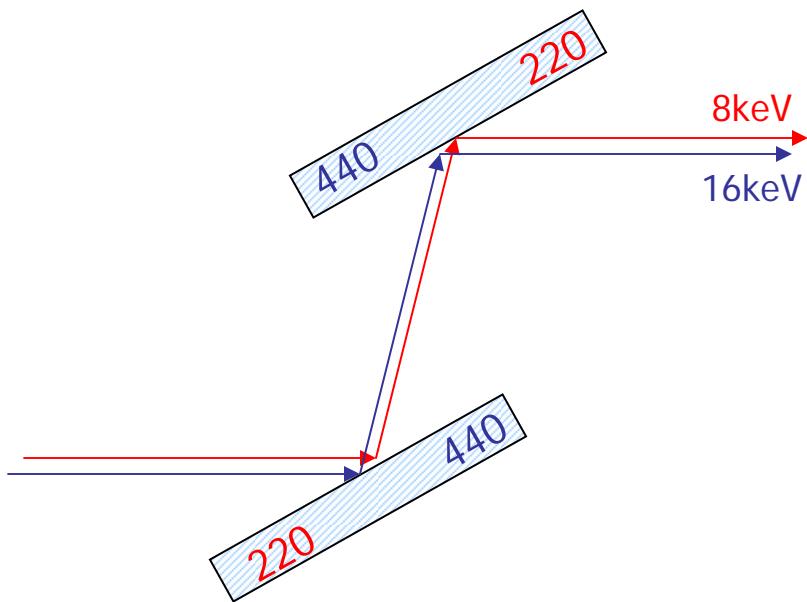
Increasing Energy Resolution



Use Collimated Beam

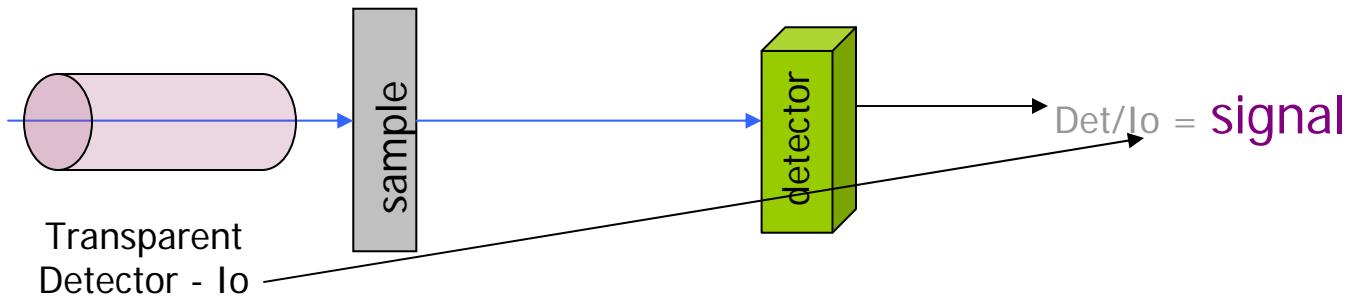
# Double Crystal Monochromator

Harmonics Rejection





# Why Harmonics are a Problem

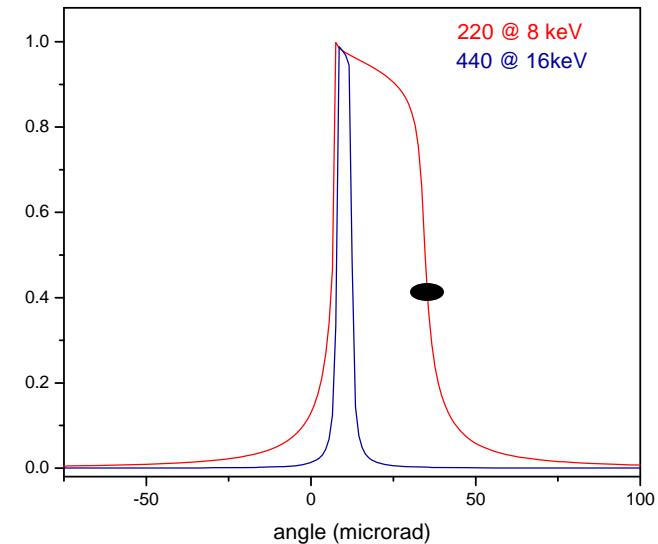
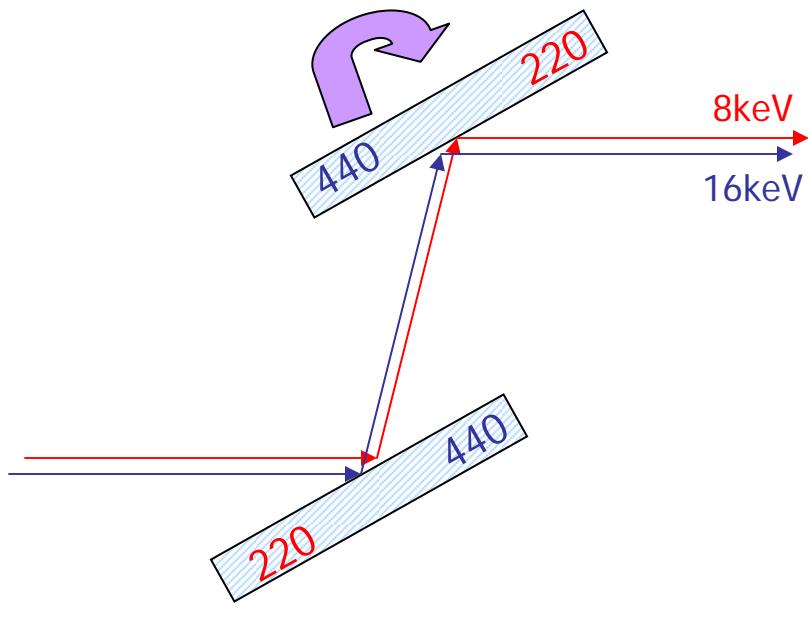


$$\text{Required Measurement} = \frac{\text{Det}_F}{I_{O_F}}$$

$$\text{Actual Measurement} = \frac{\text{Det}_F + \text{Det}_H}{I_{O_F} + I_{O_H}}$$

# Double Crystal Monochromator

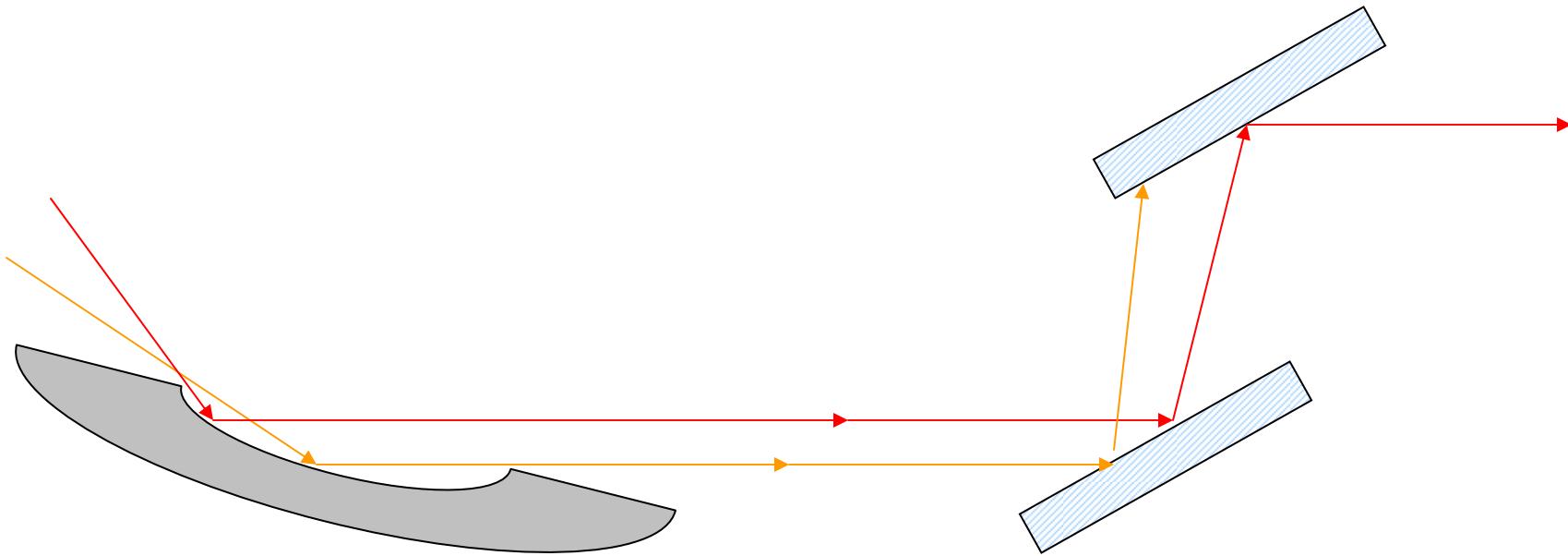
## Harmonics Rejection



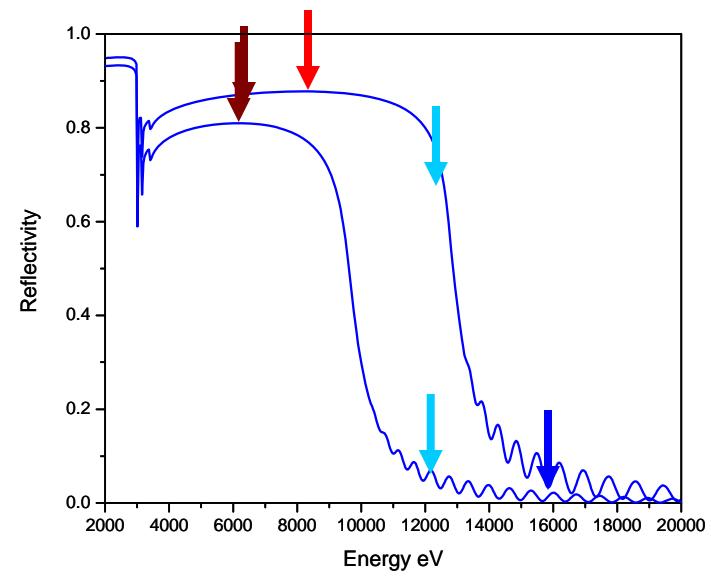
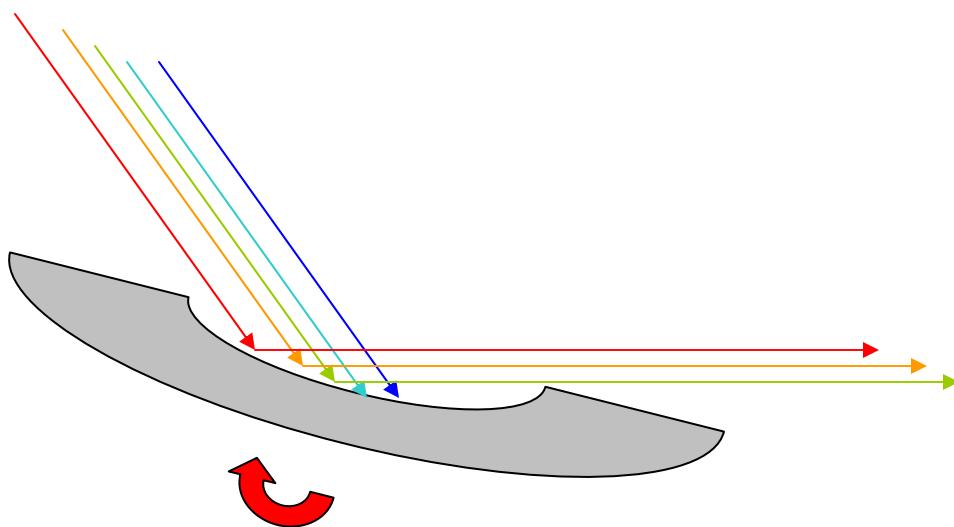
*detuning*

# Double Crystal Monochromator

## Collimating mirror for Harmonic Rejection



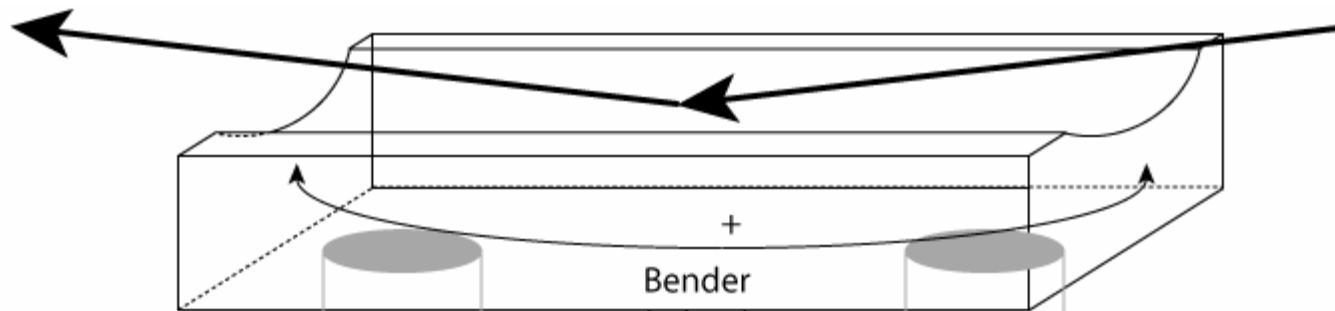
# Harmonic Rejection Mirror



Ni kedge  
Mn kedge



# Focusing Mirror



A Cylindrical Mirror Bent into a Torous

Focuses Vertically and Horizontally



# XAS BL Optics Layout

Bend Magnet or  
Wiggler Preferred.

Undulator – should  
be scanned.

Storage ring with  
straight sections

insertion device

Mo Slits

Collimating/ Harmonic  
Rejection Mirror

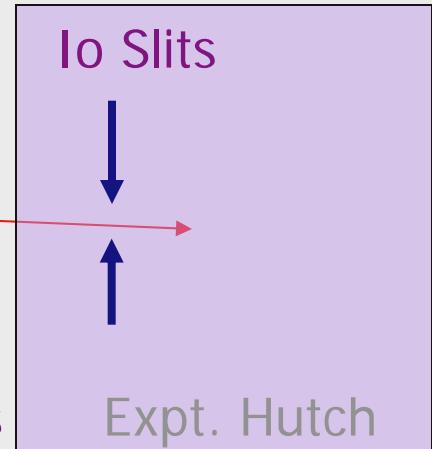
Double Crystal  
Monochromator

Mono Slits

Focusing  
Mirror

M1 Slits

"Detune"



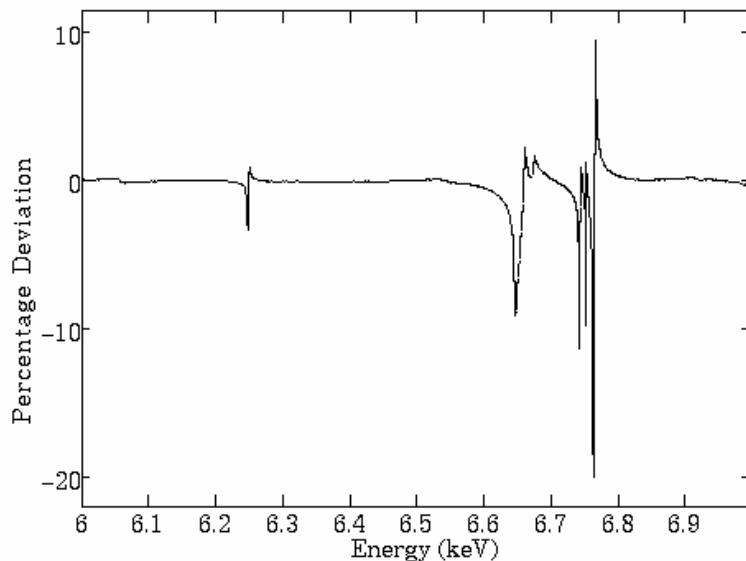
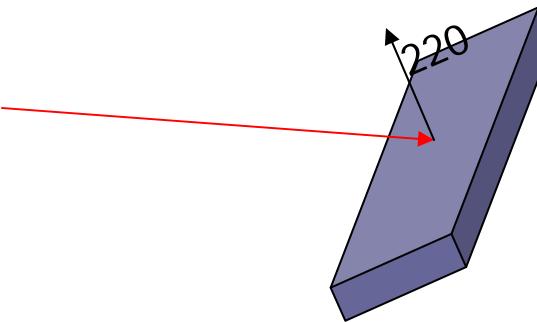
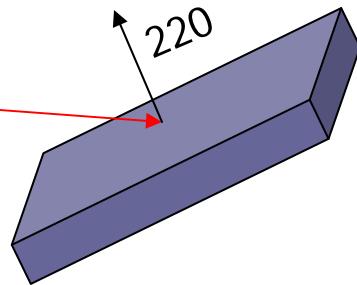
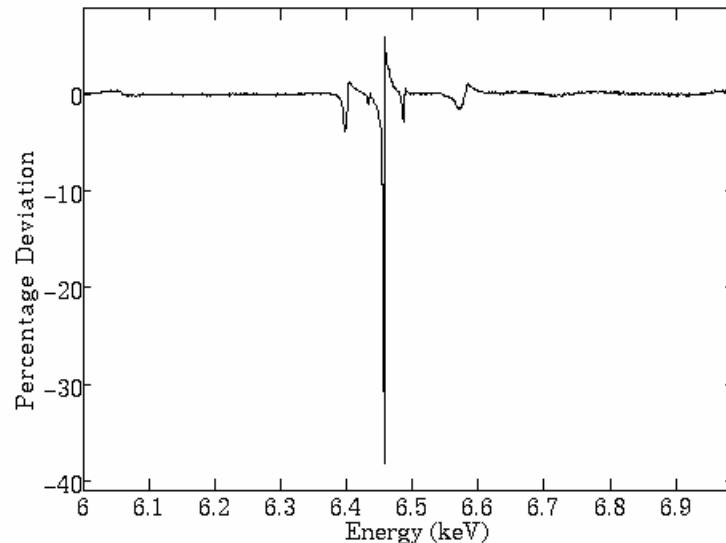
1. Energy Resolution
2. Harmonic Rejection
3. High Flux Density

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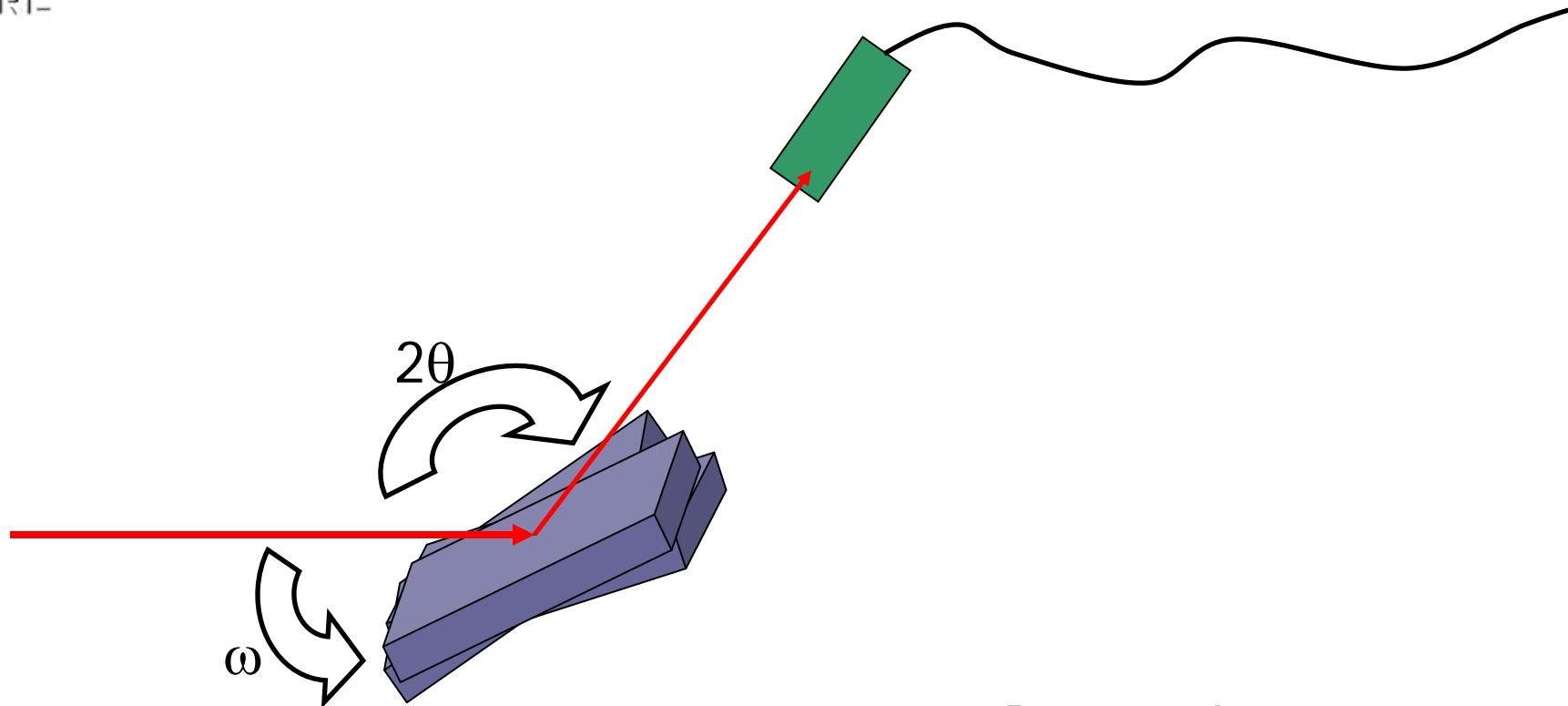




# Monochromator “Glitches”

Si(220)  $\phi=0^\circ$     6- 7 keVSi(220)  $\phi=90^\circ$     6- 7 keV

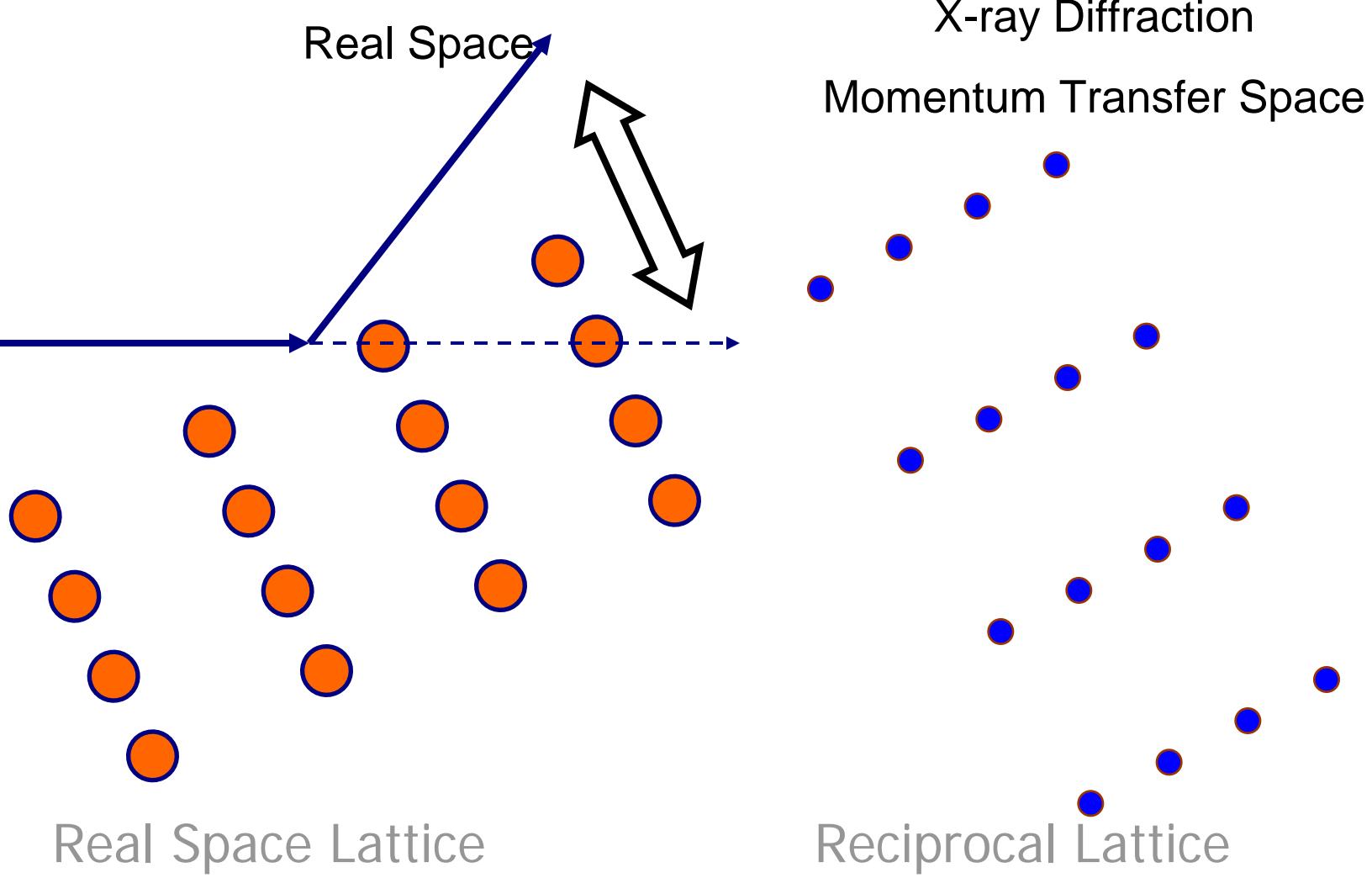
# Scattering from a Single crystal



Bragg's Law:

$$2d \sin(\theta) = h/E$$

# Scattering from a Single crystal

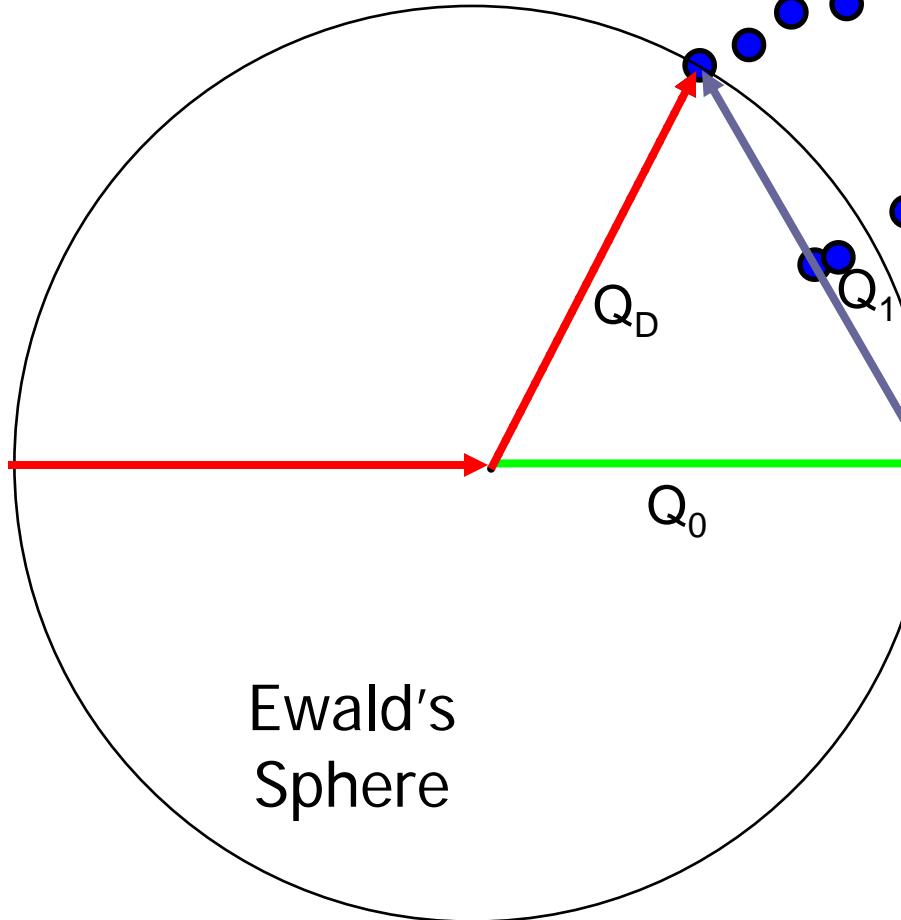


# Scattering from a Single crystal

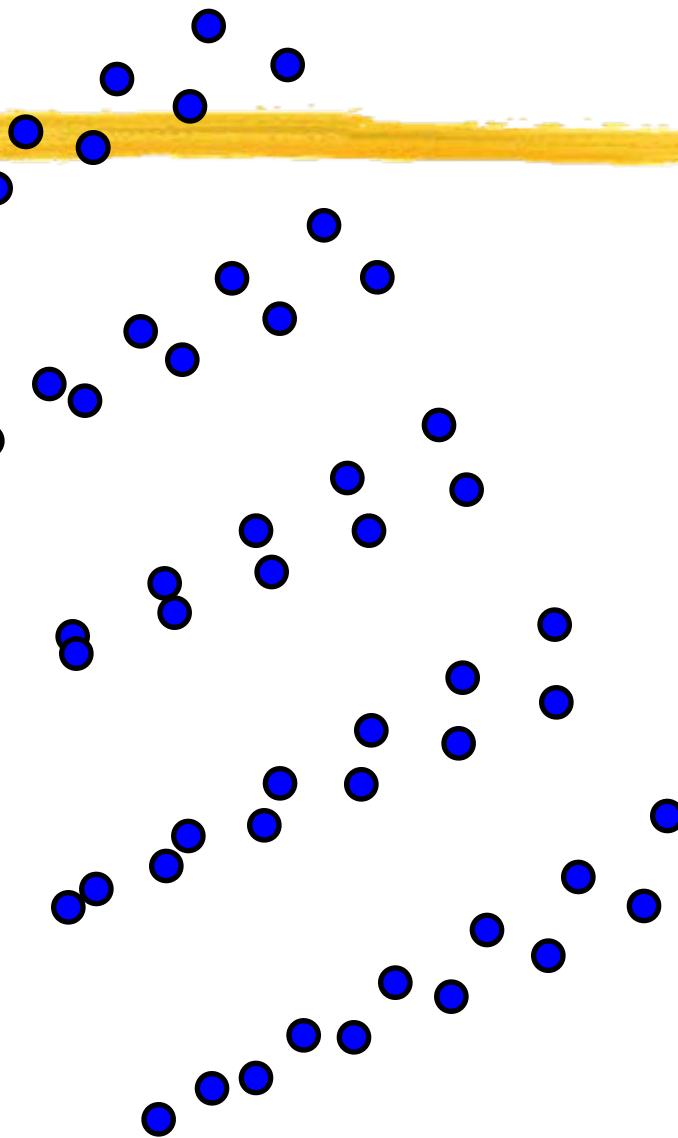
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SSRL

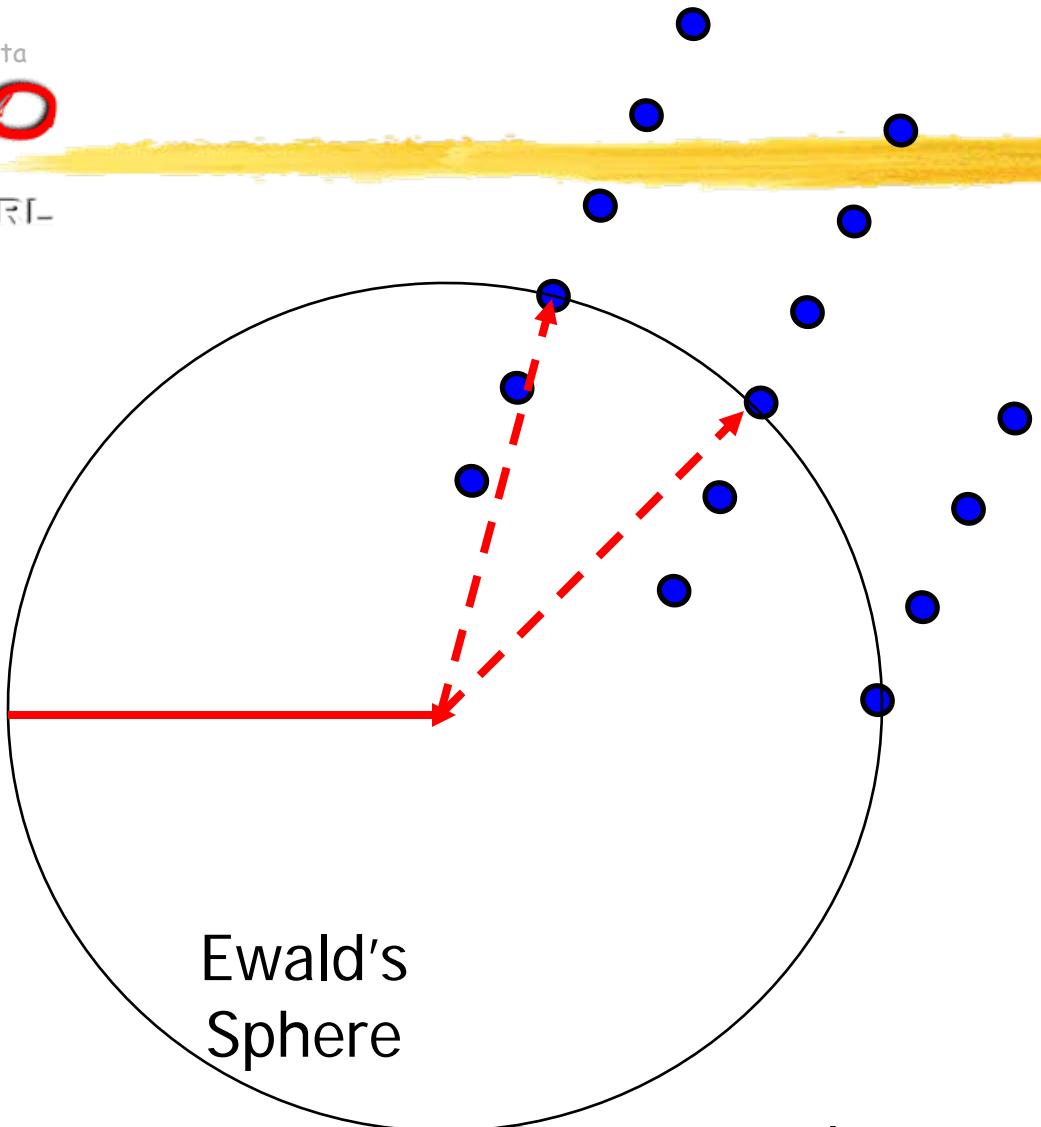


Ewald's  
Sphere



# Multiple Reflections

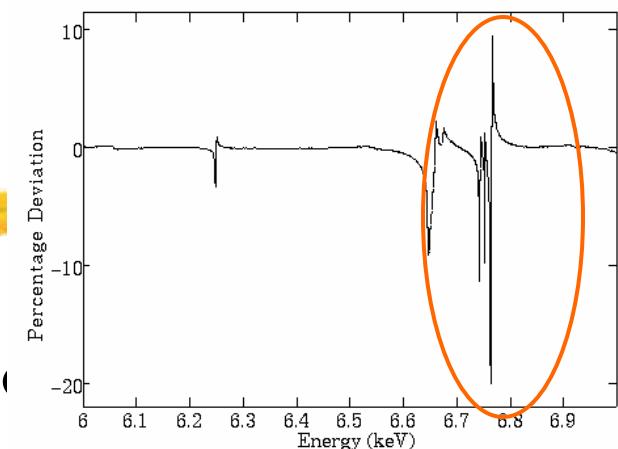
Si(220)  $\phi=0^\circ$  6-7 keV



Ewald's  
Sphere

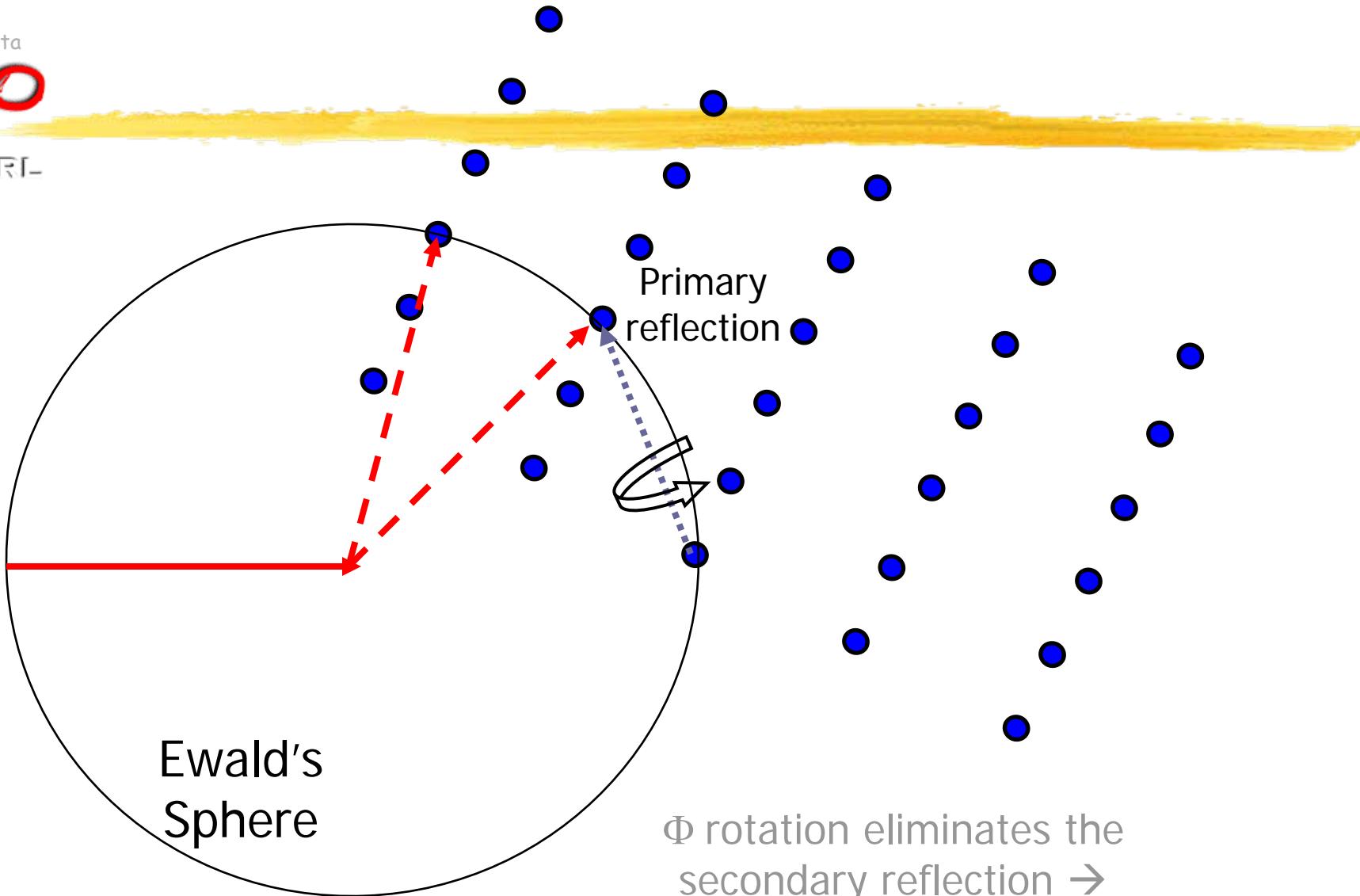
Resonance between  
the two reflections

Energy Transfer  
between the two



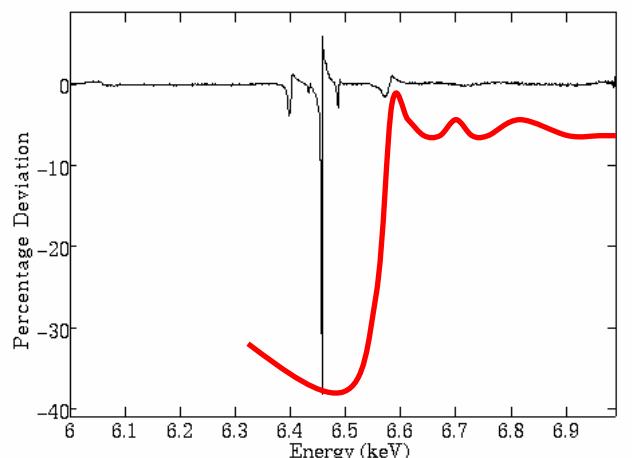
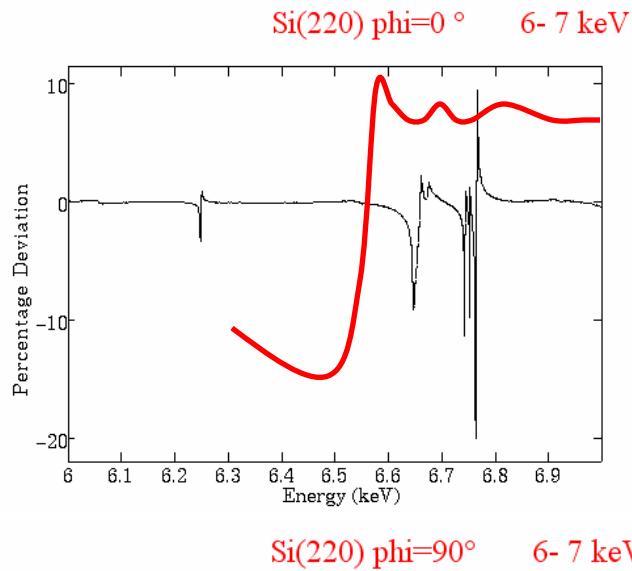
# Multiple Reflections – Phi Rotation

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$\Phi$  rotation eliminates the  
secondary reflection →  
eliminates the resonance/glitch

# Monochromator “Glitches”



- ◆ Location Depends on Phi Orientation
- ◆ Severity depends on precise crystal orientation, difficult to predict
- ◆ Can not be eliminated, but sometimes can be made sufficiently narrow by slits adjustment that EXAFS are not affected.

# Preparation for an XAS Experiment

## ◆ Absorbing Element

- ◆ K, L, M edge
- ◆ BL with the appropriate energy range

## ◆ Energy Resolution

- ◆ Monochromator crystal order (e.g., 111, 220)
  - ◆ Crystal Orientation – phi cut – “Glitch” spectrum.
- ◆ Close Slits
- ◆ Collimation of the beam prior to the Mono

XANES

## ◆ Harmonic Rejection Strategy

- ◆ Mo angle adjustment for appropriate cut-off
- ◆ Detune the monochromator

## ◆ Flux Density on the sample

- ◆ Select an insertion device source if available
- ◆ Adjust the M1 focus
- ◆ Lower Order Monochromator Crystal
- ◆ Open Slits

EXAFS



# XAS BL Optics Layout

Bend Magnet or  
Wiggler Preferred.

Undulator – should  
be scanned.

Storage ring with  
straight sections

insertion device

Mo Slits

Collimating/ Harmonic  
Rejection Mirror

Double Crystal  
Monochromator

Focusing  
Mirror

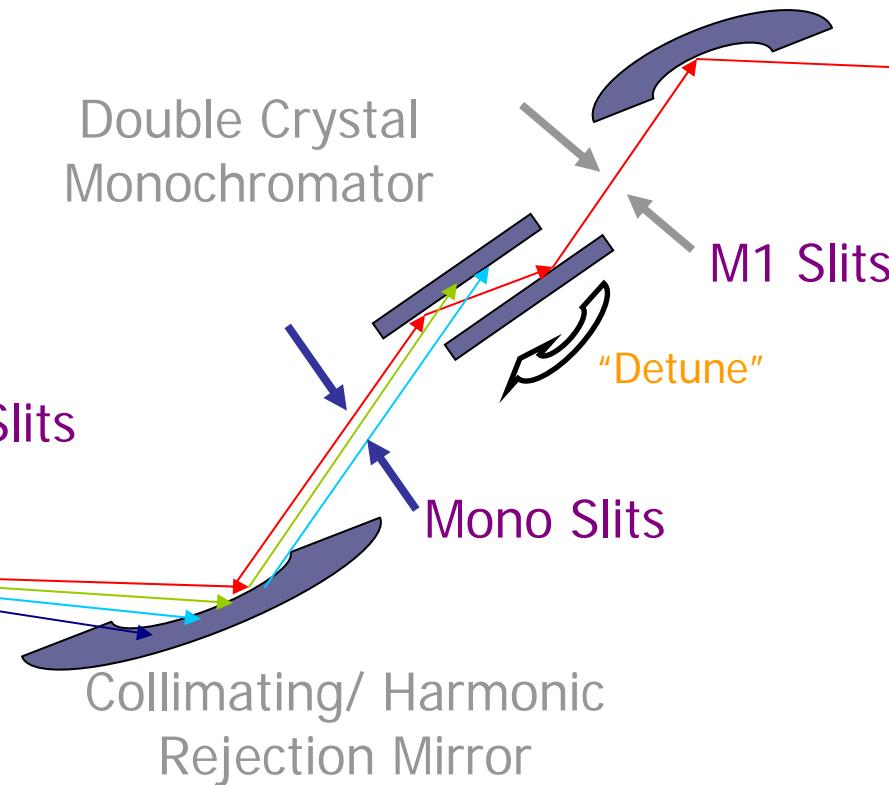
M1 Slits

"Detune"

Mono Slits

Io Slits

Expt. Hutch



# Thanks

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## Questions?



*Stanford Synchrotron Radiation  
Laboratory*



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