Materials Characterization using X-ray Scattering & Fluorescence

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N.S.LS

- structure
- Evolution of structure as a fn. of P.T. etc.
- Elementary Excitations

Compton Scattering
Diffuse Scattering
Resonant X-ray Scattering
Small angle scattering
Inelastic x-ray scattering
Surface, Interfaces Scattering

- $< 3000\,eV \sim > 100\,keV$
- High flux e.g. 10^{12} photons/sec
  Si(111) Mono.
- Large dynamic range
- Combining spectroscopy with scattering

Detectors Currently Used

* Whatever We Can Buy *

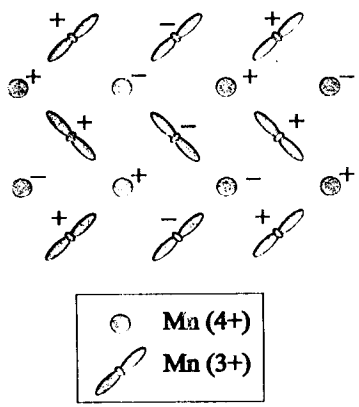
Hard X-Ray :
- * Photodiodes
- APD
- * Ion chambers
- * NaI
- * Si(Li), Ge
- * Amptek / PIN diode
- gas proportional counter (1D/2D)
- CCD

Soft X-ray :
- * photodiodes
- gas proportional counter
- Ge(Li)
- * Electron multiplier / channel plate

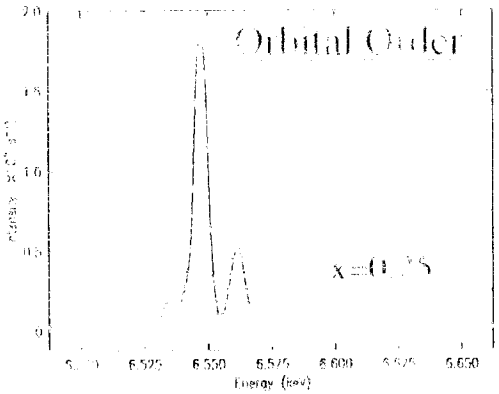
⇒ "Optimize Detector for the Experiment"

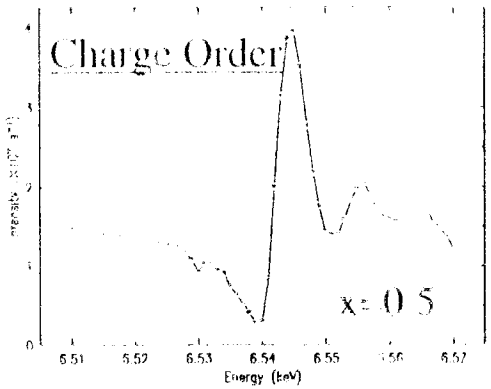
Resonant scattering from Spin, Orbital and Charge Order in Transition Metal Oxides

Manganites

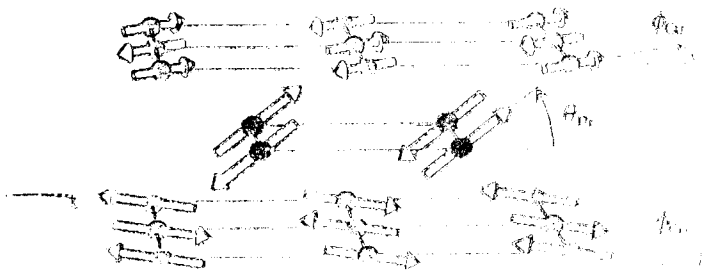


Resonant scattering at Mn K-edge



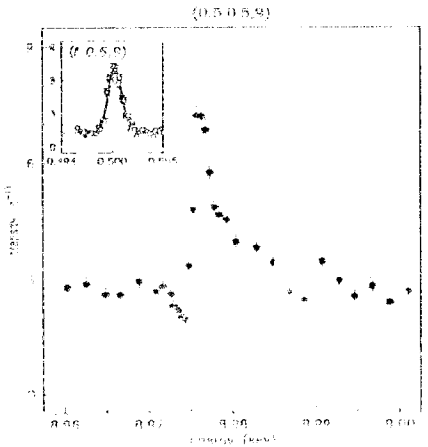


Cuprates

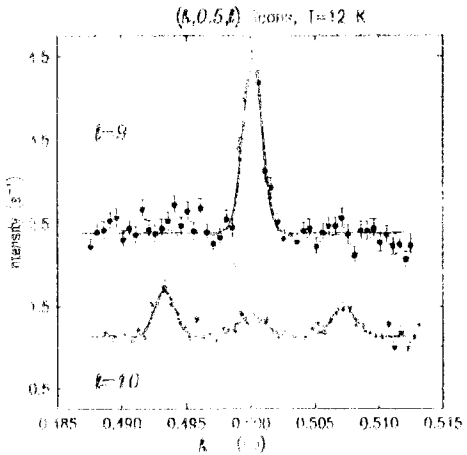


AFIII phase

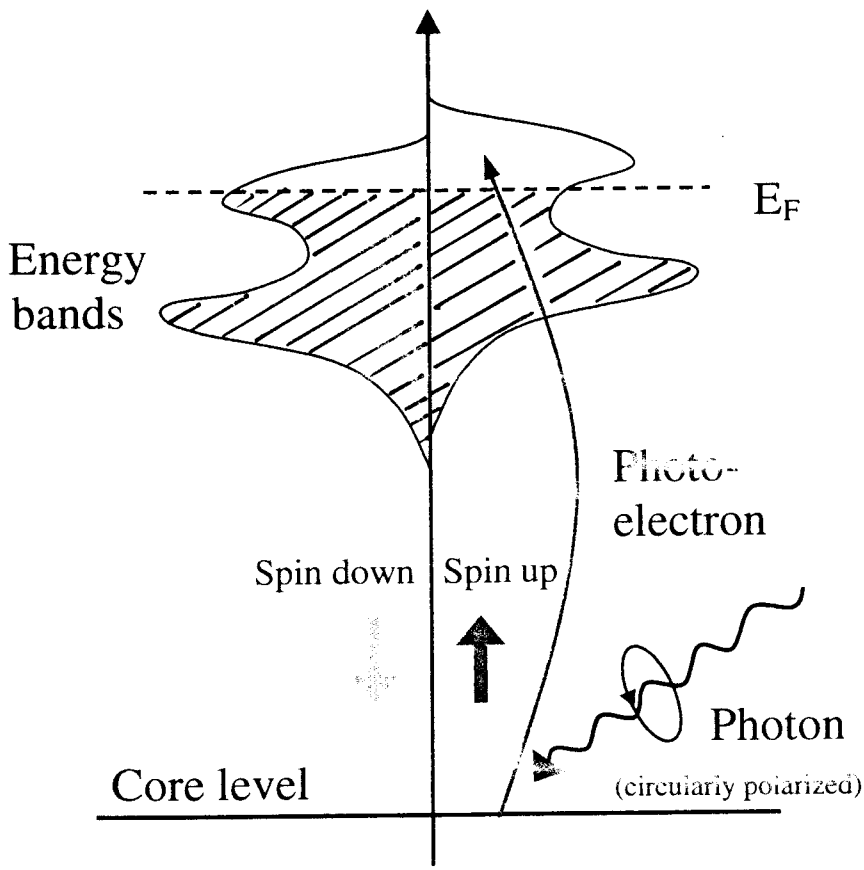
Magnetic scattering at Cu K-edge



ESRF data



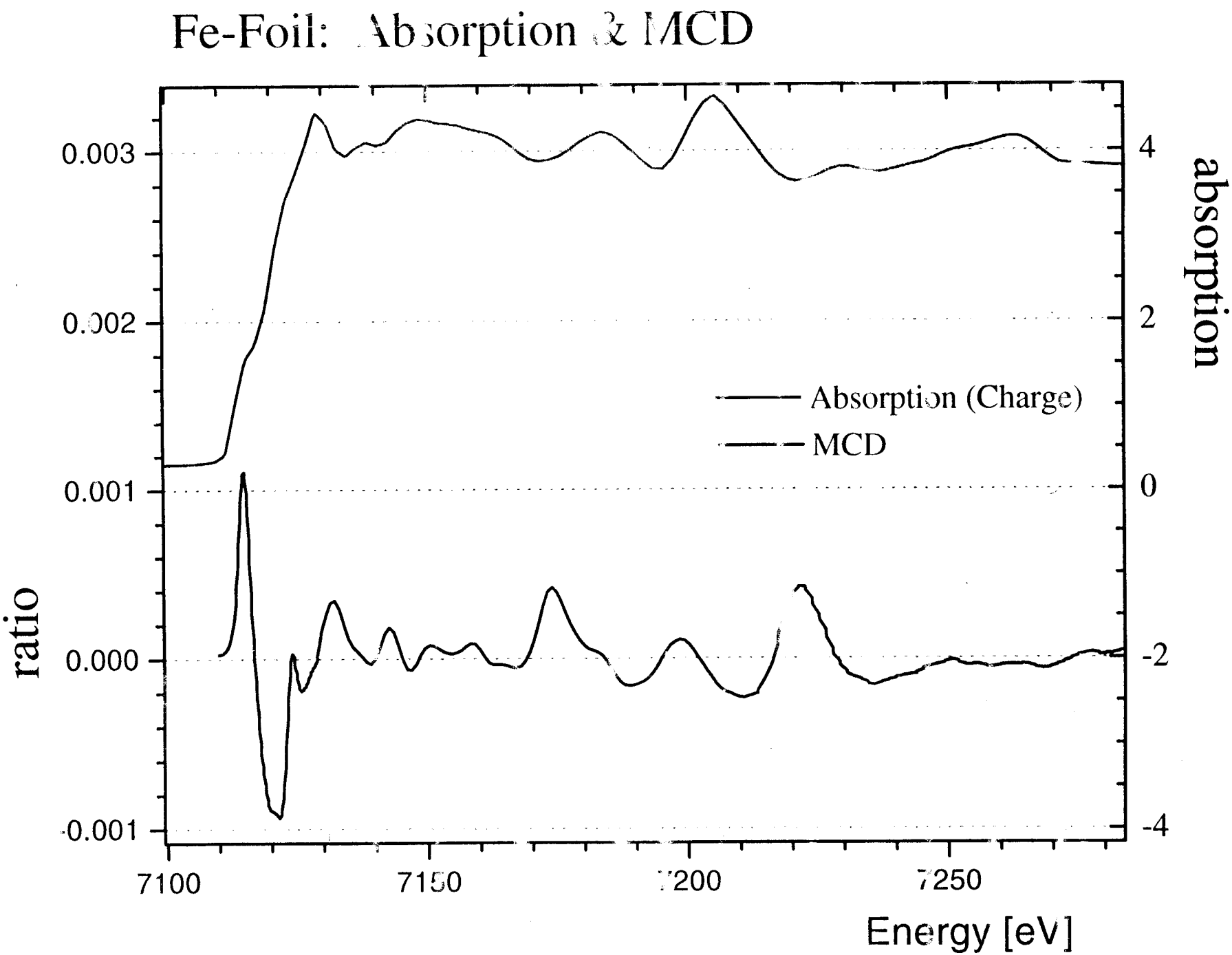
Magnetic Circular Dichroism (MCD)



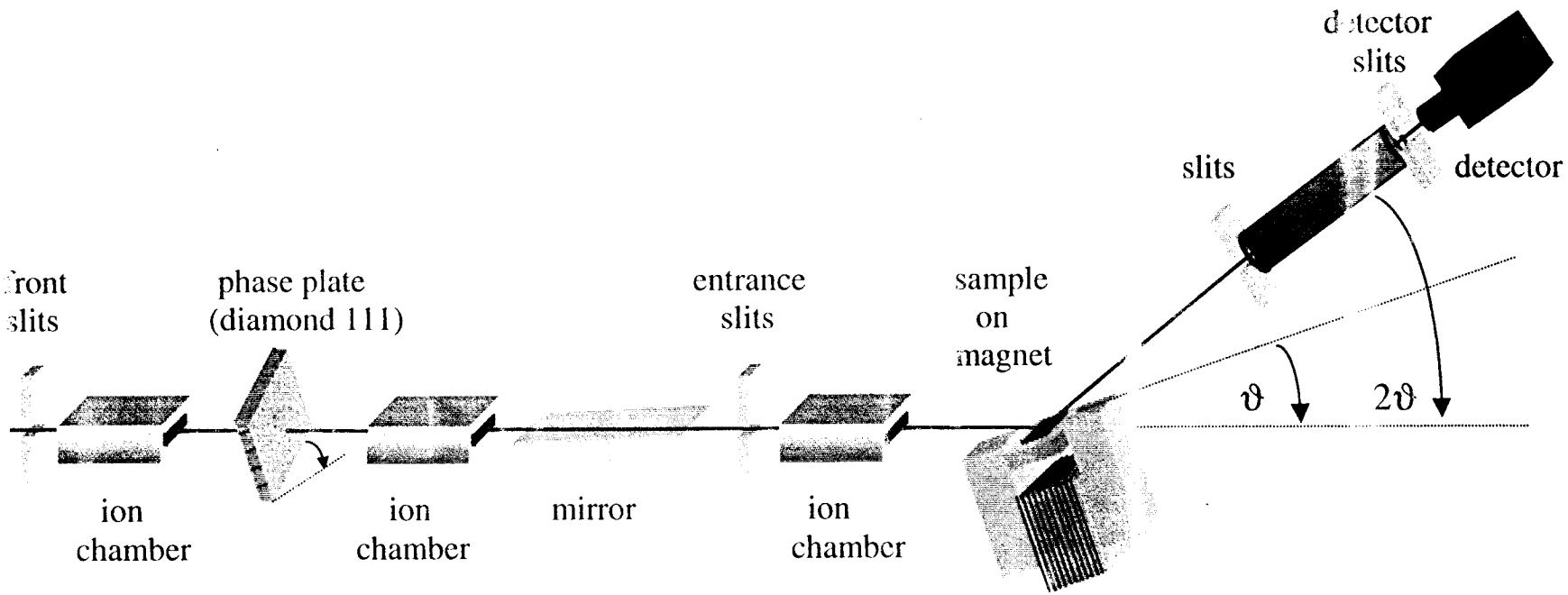
Splitting of the valence states due to magnetization
⇒ Absorption of left- and right- circularly polarized x-rays are different (**MCD-Effect**).

$$\Delta I = I_{\uparrow\uparrow} - I_{\uparrow\downarrow} \neq 0 \qquad \left(\frac{\Delta I}{2I} \approx -P_c' \cdot \mu_c \cdot t \right)$$

$I_{\uparrow\uparrow}$: Magnetization ↑↑ Helicity of photon beam
$I_{\uparrow\downarrow}$: Magnetization ↑↓ Helicity of photon beam


Fe-Foil: Absorption & MCD
0.003
0.002
0.001
0.000
-0.001
ratio
4
2
0
-2
-4
absorption
Absorption (Charge)
MCD
7100
7150
7200
7250
Energy [eV]

Reflectivity at CMC-CAT Beamline, APS, Argonne

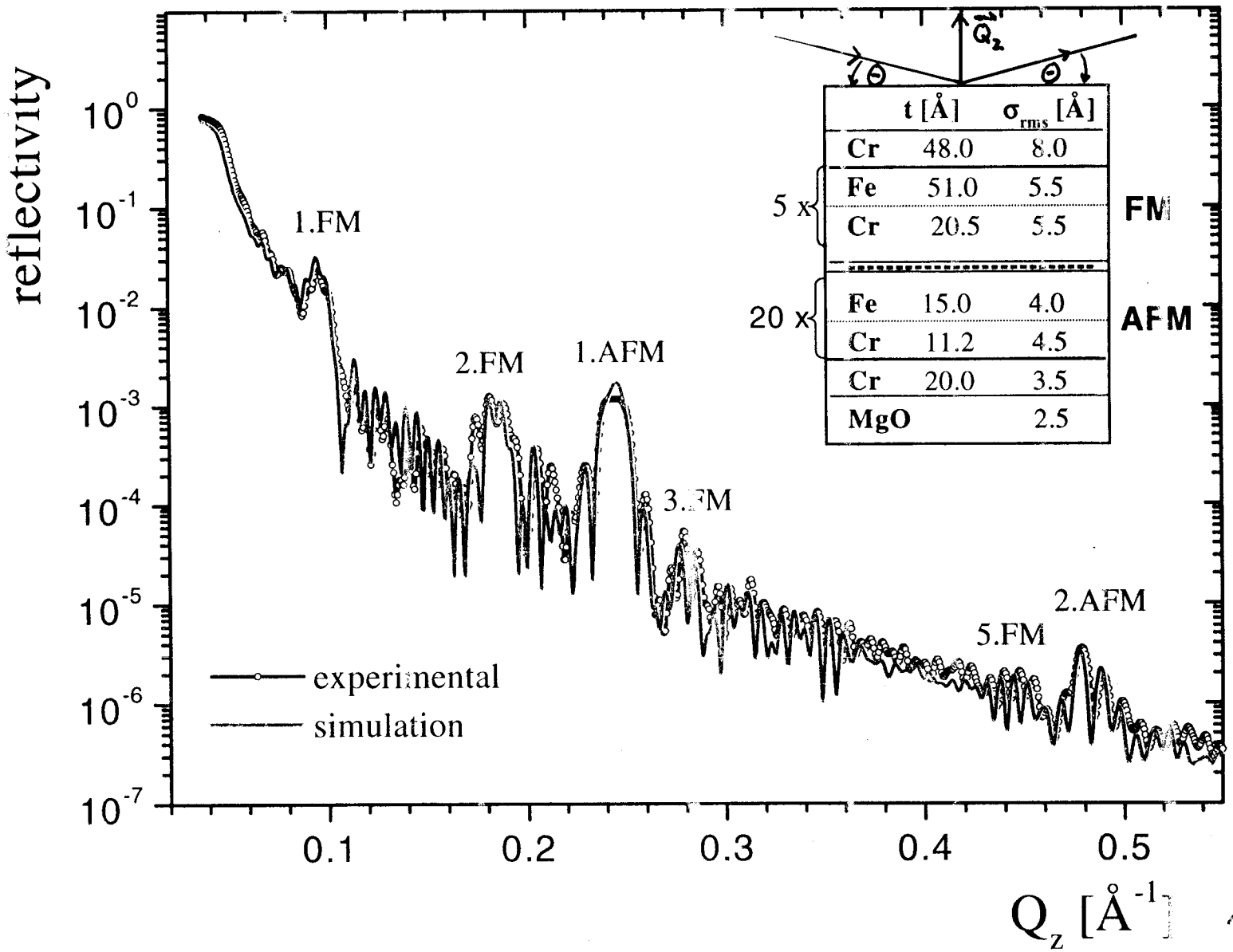


- degree of **Circular Polarization** (MCD on Fe-Foil): ≈ **65 %**
- **Flux** (slits: 1 mm (v) × 2 mm (h)): **$0.9 \cdot 10^{12}$ circularly polarized photons/sec**

Specular Reflectivity (Charge!)

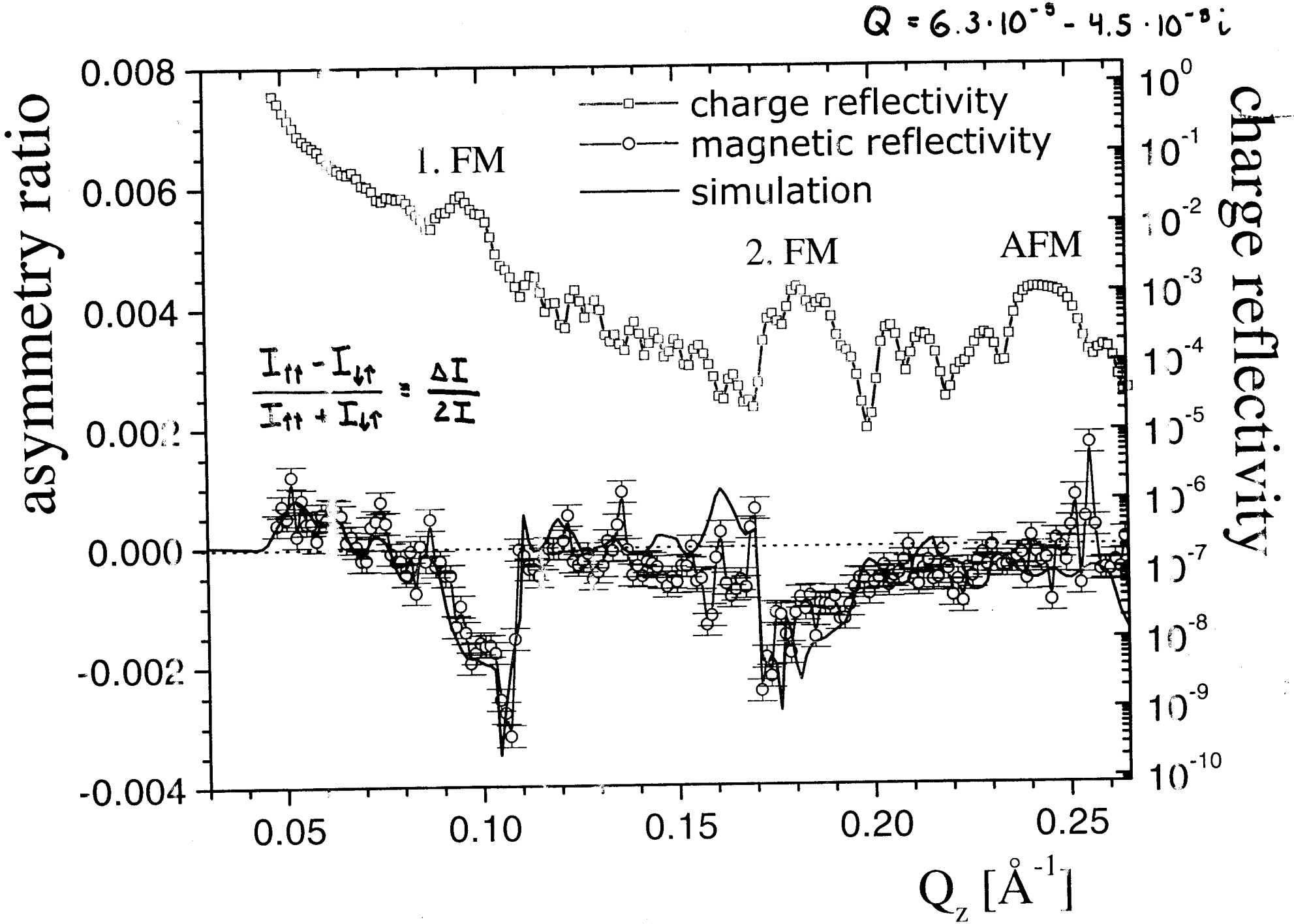
[FeCr]-multilayer data+simulation

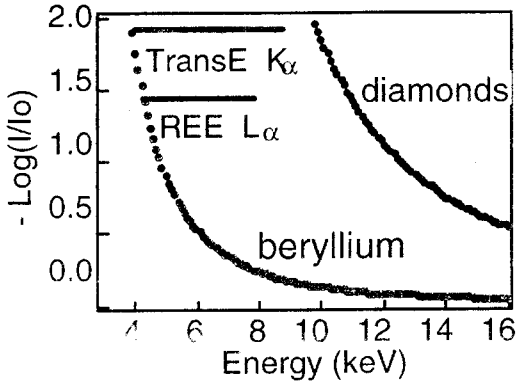
7100 eV

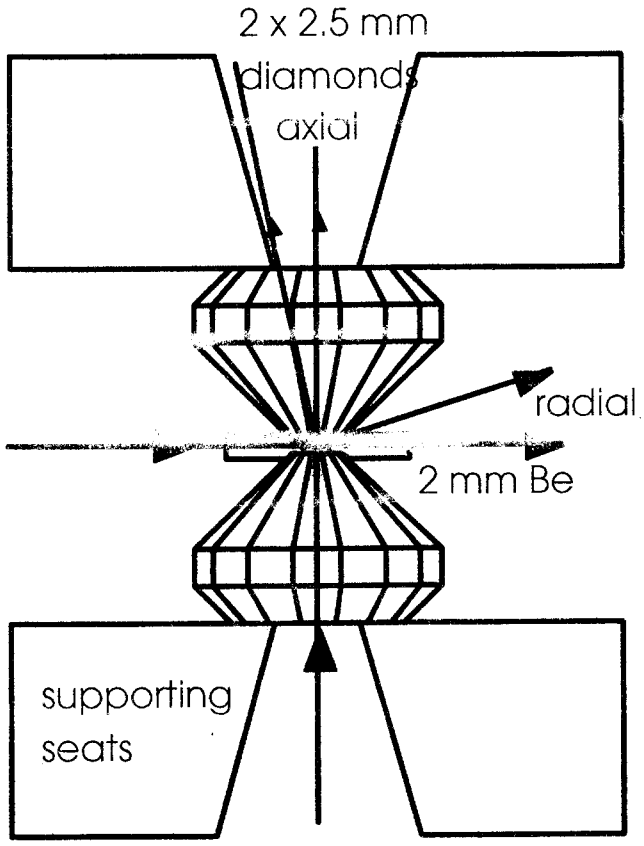


	t [Å]	σ_{rms} [Å]	
Cr	48.0	8.0	
5 x { Fe	51.0	5.5	FM
5 x { Cr	20.5	5.5	FM
20 x { Fe	15.0	4.0	AFM
20 x { Cr	11.2	4.5	AFM
Cr	20.0	3.5	
MgO		2.5	

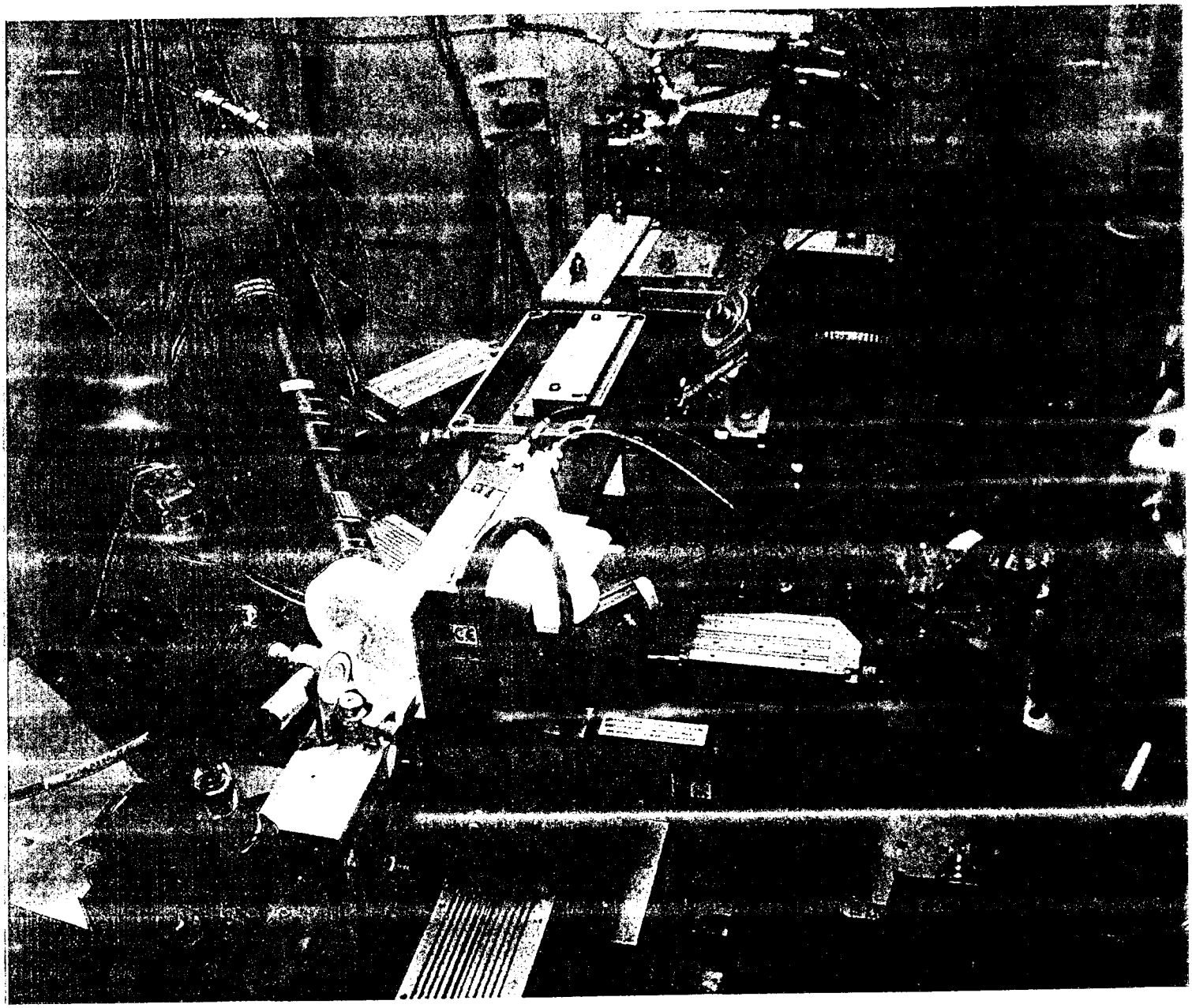
$\sim \sin\Theta$


Q = 6.3·10^-5 - 4.5·10^-8 i
charge reflectivity
magnetic reflectivity
simulation
1. FM
2. FM
AFM
$\frac{I_{\uparrow\uparrow} - I_{\downarrow\uparrow}}{I_{\uparrow\uparrow} + I_{\downarrow\uparrow}} = \frac{\Delta I}{2I}$
asymmetry ratio
charge reflectivity
0.008
0.006
0.004
0.002
0.000
-0.002
-0.004
0.05
0.10
0.15
0.20
0.25
Q_z [Å^{-1}]
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}

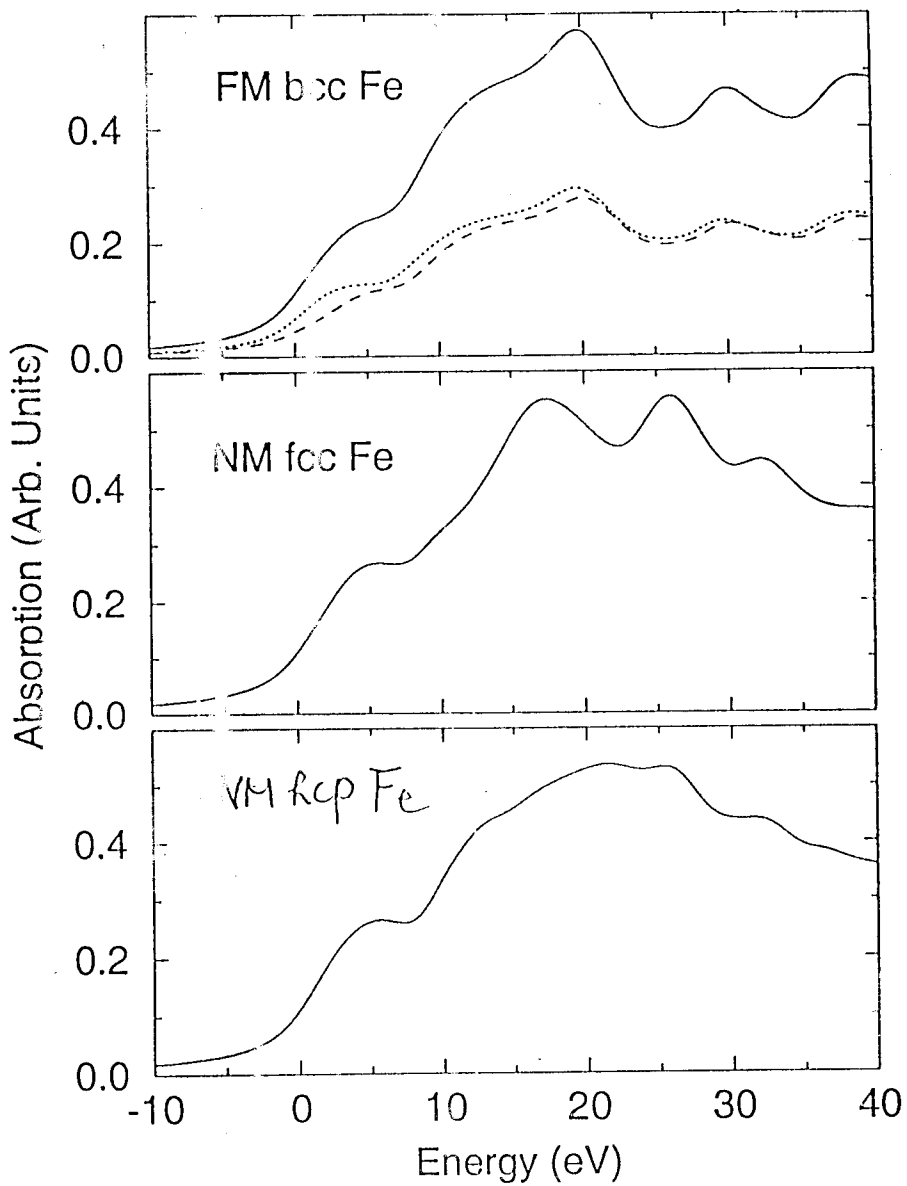

2.0
1.5
1.0
0.5
0.0
- Log(I/Io)
TransE Kα
REE Lα
diamonds
beryllium
4 6 8 10 12 14 16
Energy (keV)

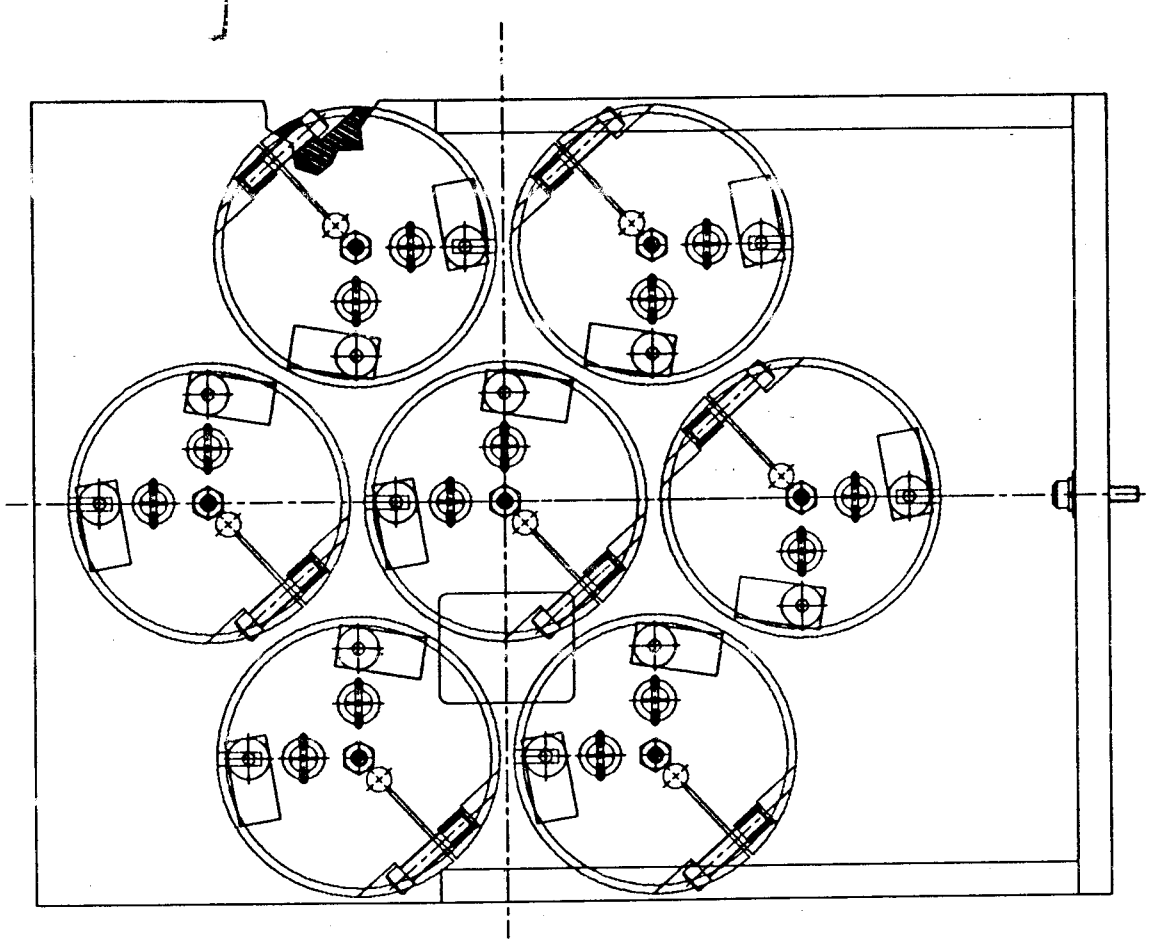

2 x 2.5 mm
diamonds
axial
radial
2 mm Be
supporting
seats

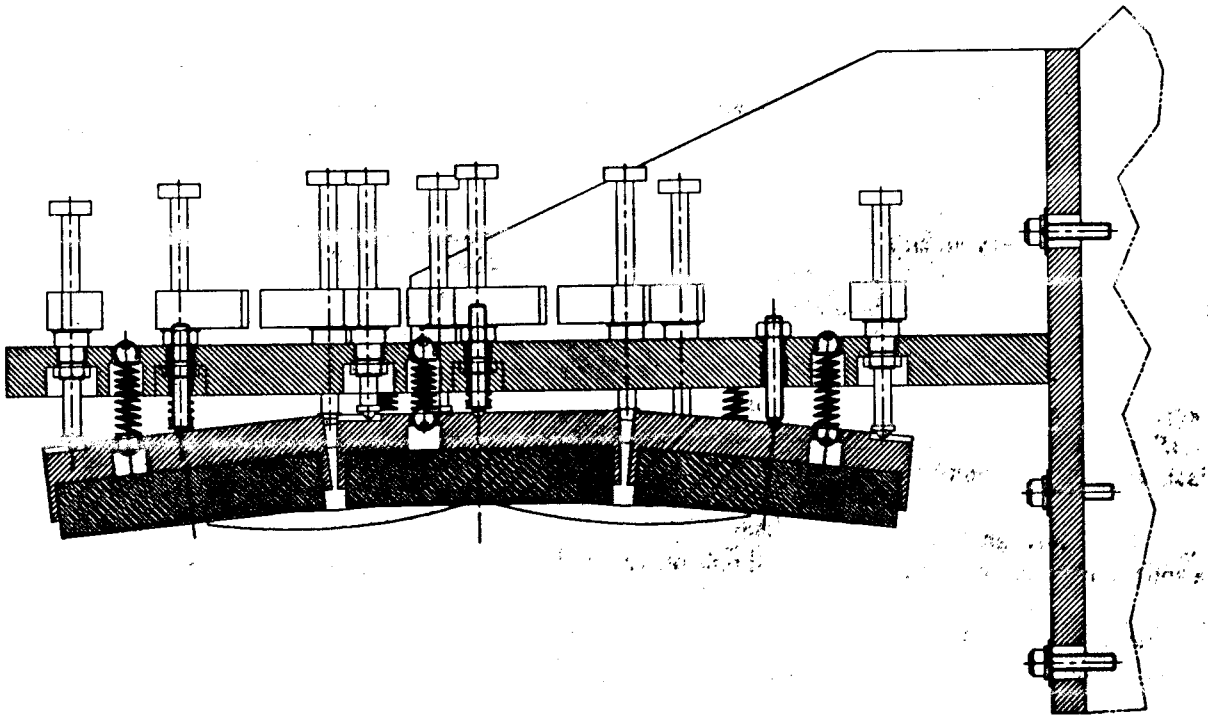
Mao

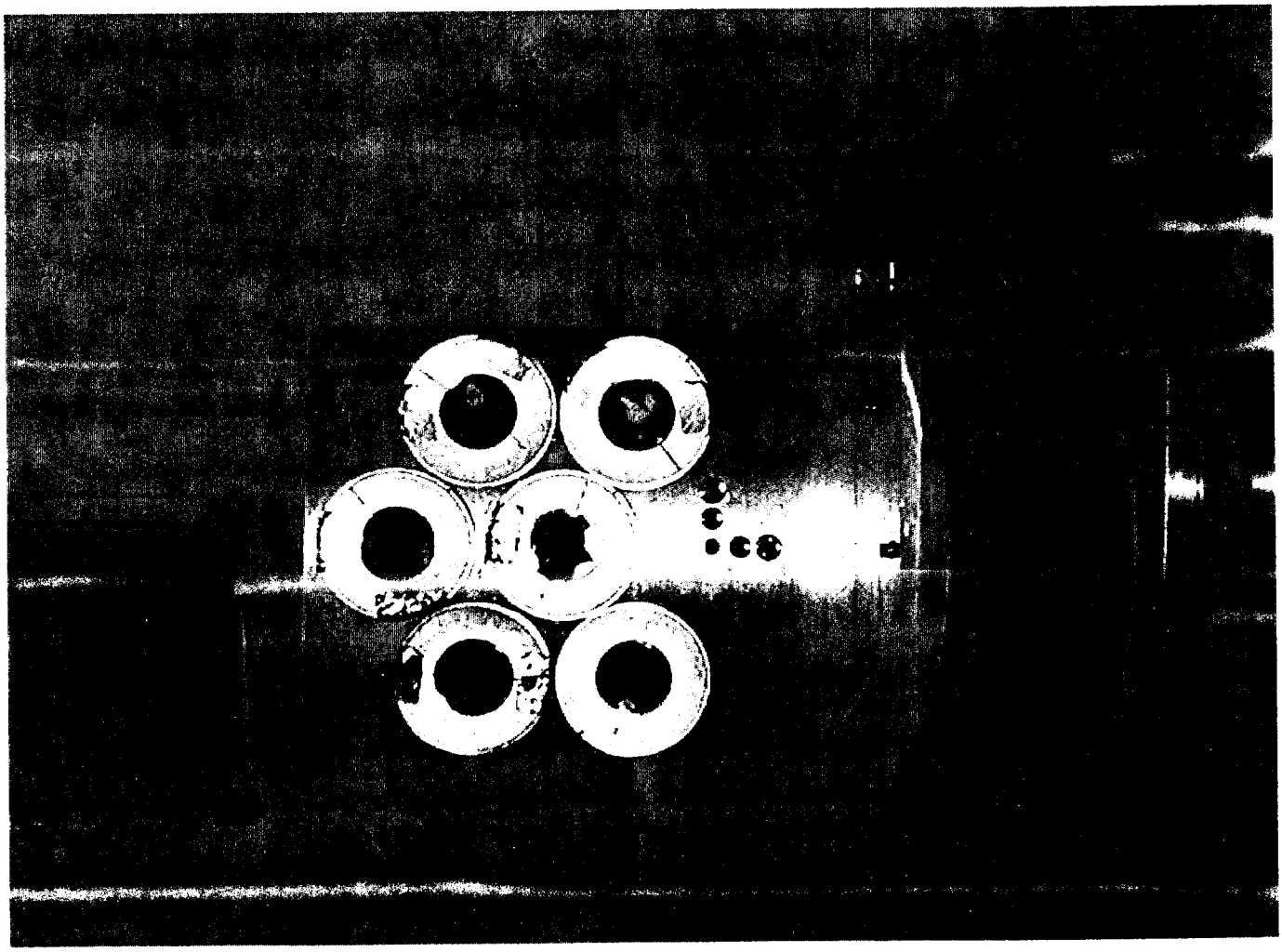


Fe K edge X-ray Absorption Spectra

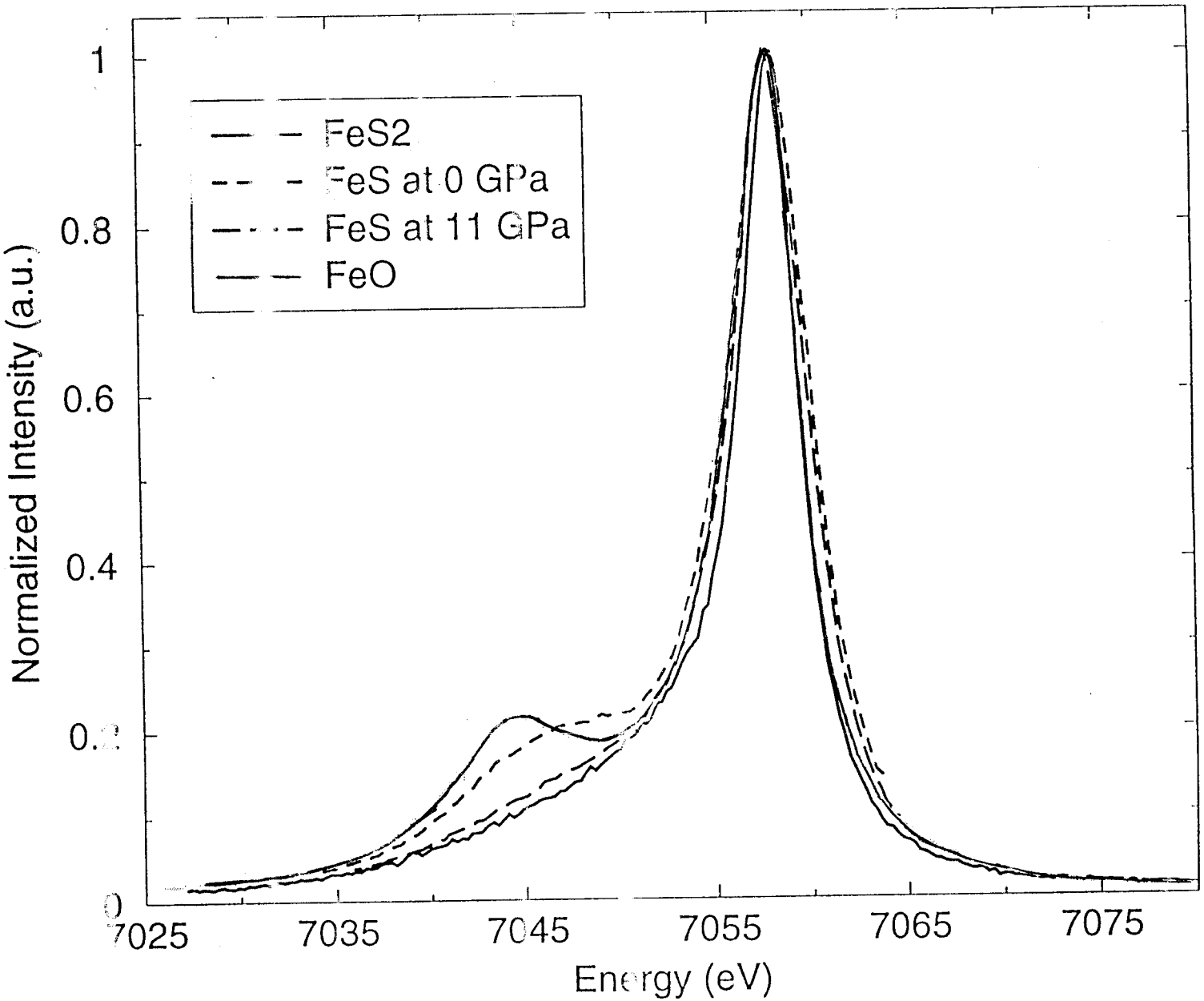




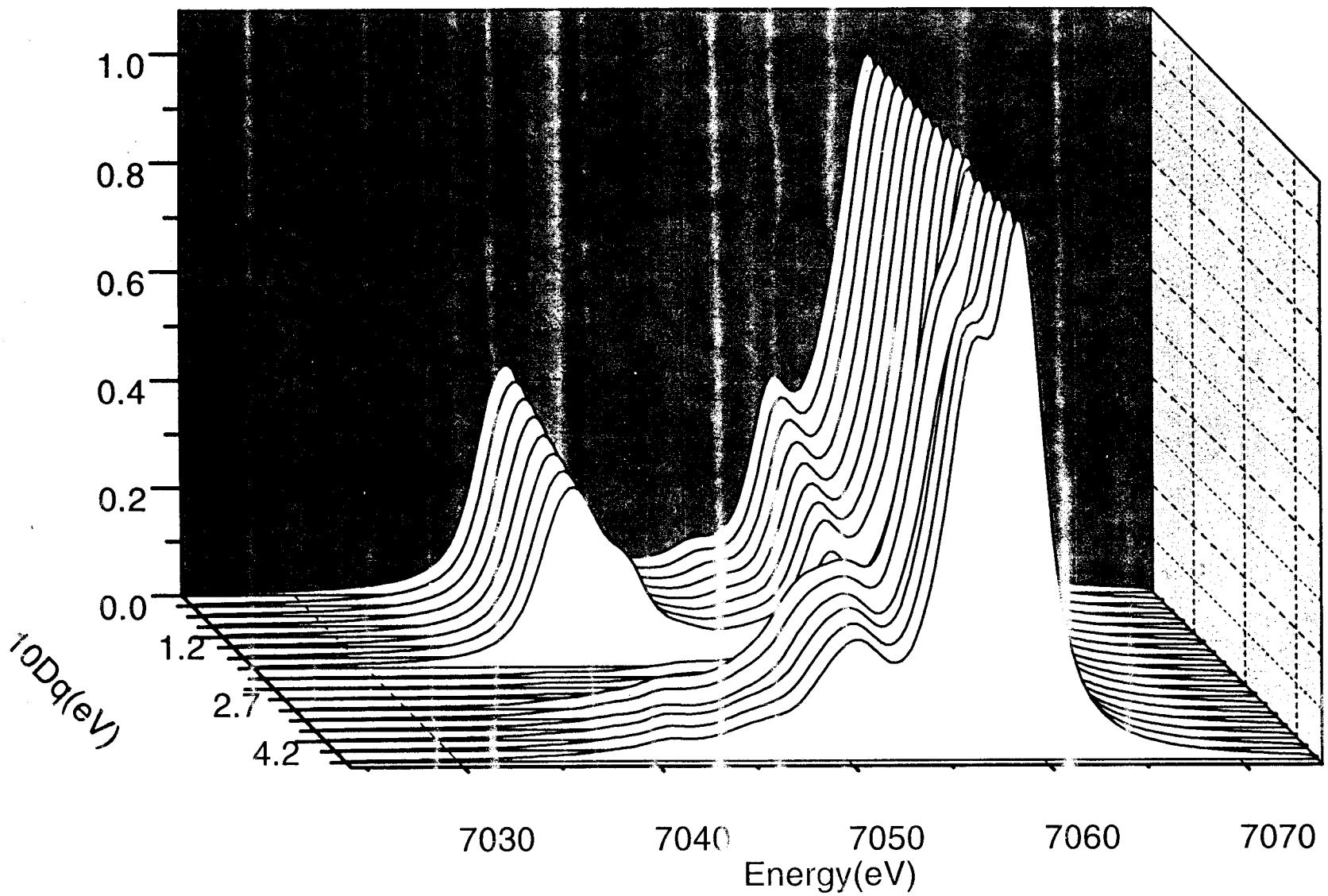




PRL 82, 3284 (1999)



Fe^{2+}, 80% Slater Integral Scaling



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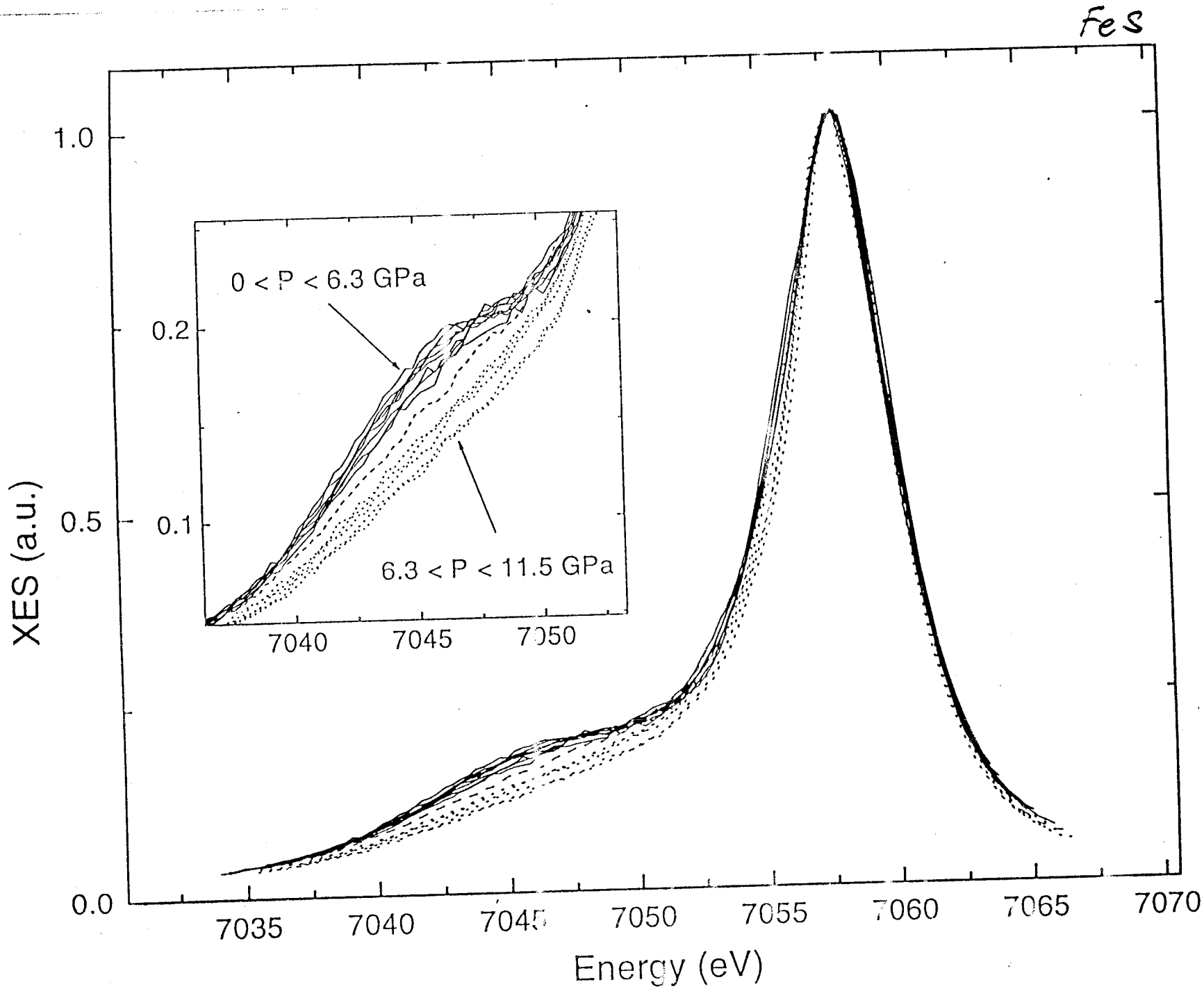
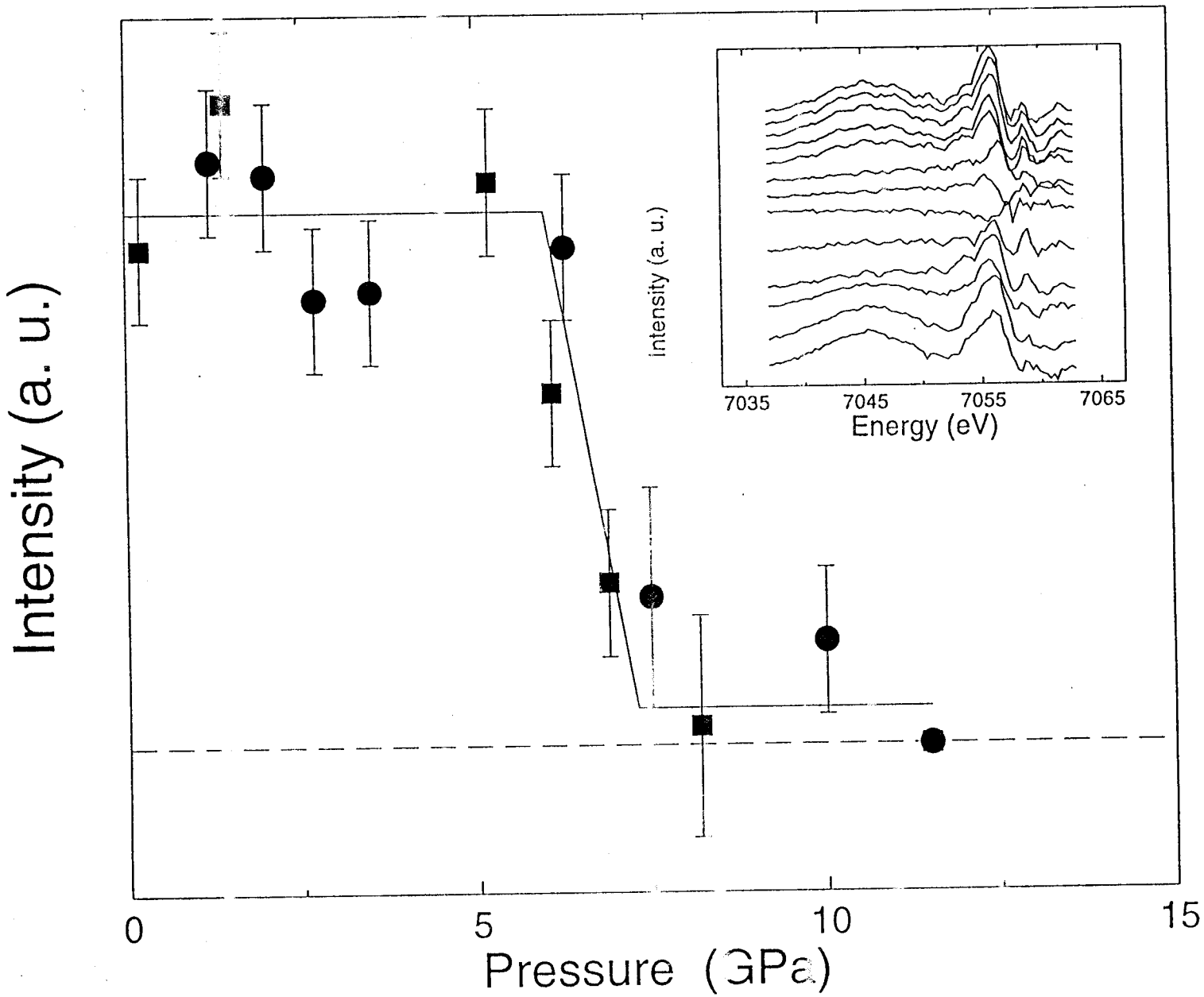

FeS
XES (a.u.)
1.0
0.5
0.0
0.2
0.1
0 < P < 6.3 GPa
6.3 < P < 11.5 GPa
7040
7045
7050
7035
7040
7045
7050
7055
7060
7065
7070
Energy (eV)

FeS


Intensity (a. u.)
0
5
10
15
Pressure (GPa)
Intensity (a. u.)
7035
7045
7055
7065
Energy (eV)