

# WINTER SCHOOL OF SYNCHROTRON RADIATION

31.01. – 04.02. 2011 Liptovský Ján,  
Slovakia

Š. Michalik: X-ray Diffraction and X-ray Absorption  
Spectroscopy in the Study of Materials with Disordered  
Structure

1 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
[www.science.upjs.sk](http://www.science.upjs.sk)



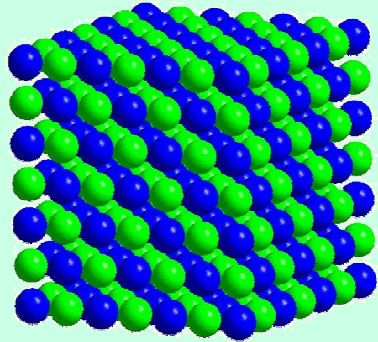
UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH  
Prírodovedecká fakulta

Múdrost' minulosti – poznatky prítomnosti – vzdelanie budúcnosti.



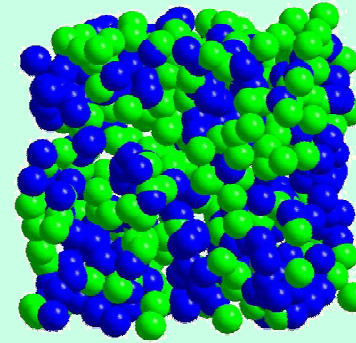
# Materials with Disordered Structure

Ordered (crystalline) structure



- periodic structure
- long range order
- symmetry

Disordered (amorphous) structure



- no periodicity
- short range order
- no symmetry

*Real life example*



2 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
www.science.upjs.sk



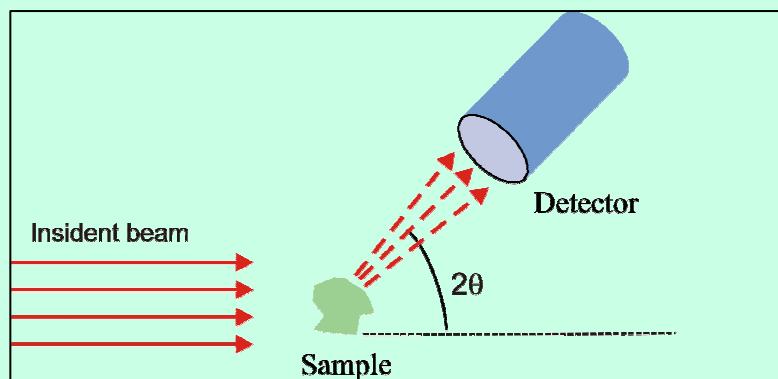
UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH

Prírodovedecká fakulta

Múdrost' minulosti – poznatky prítomnosti – vzdelanie budúcnosti.



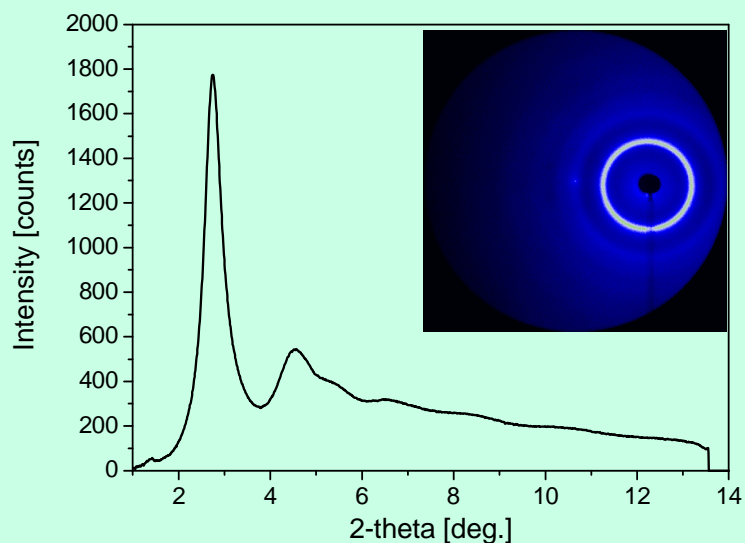
# X-ray diffraction experiments



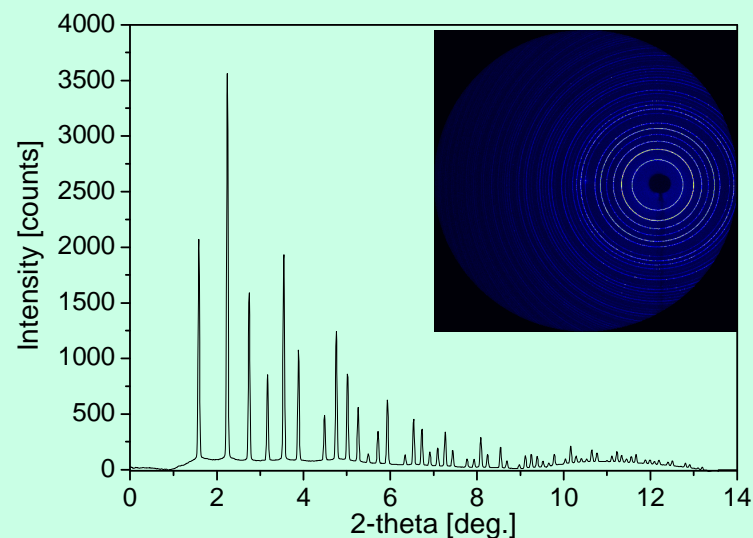
The main idea is to measure the variation in scattered intensity due to interference effects as a function of the (diffracted) angle

$$Q = \frac{4\pi}{\lambda} \sin(\theta) \quad - \text{a wave transfer vector}$$

## Amorphous material



## Crystalline material



3 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
www.science.upjs.sk



UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH

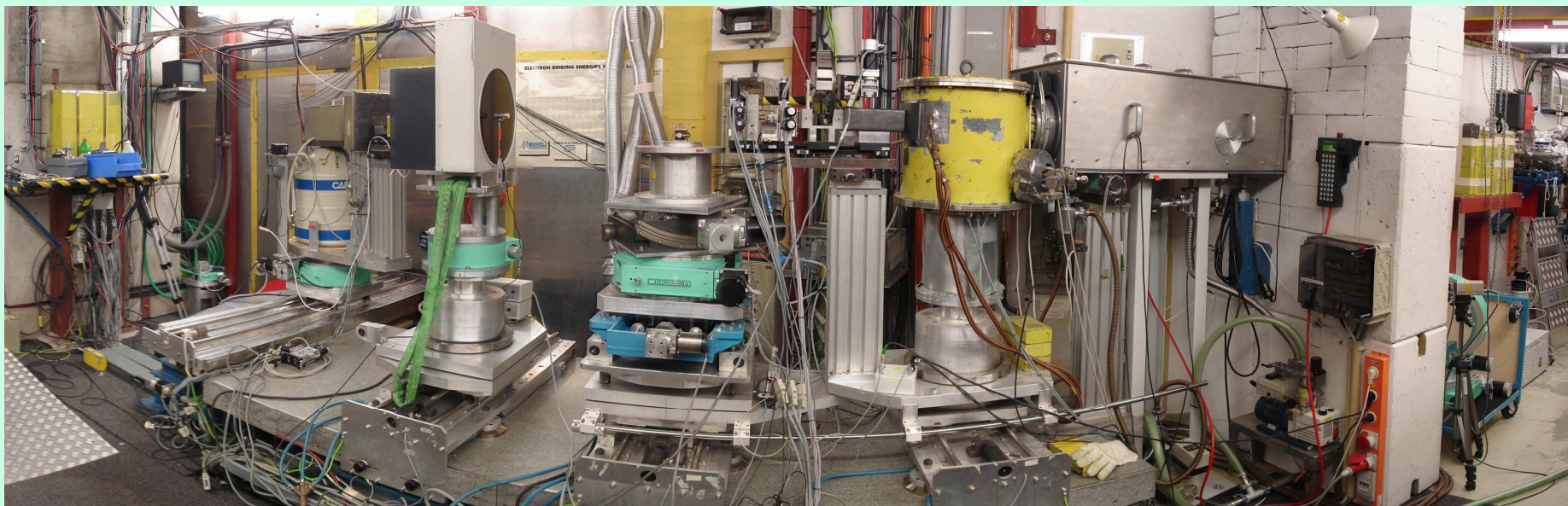
Prírodovedecká fakulta



Múdrosť minulosti – poznatky prítomnosti – vzdelanie budúcnosti.

# Experimental station BW5

BW5 is dedicated to X-ray scattering experiments at energies between **60 and 150 keV**.



Present applications are:

- charge density studies of single crystals
- structural phase transitions
- *analysis of the pair distribution function of amorphous material and liquids*
- texture analysis of powder materials

4 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
[www.science.upjs.sk](http://www.science.upjs.sk)

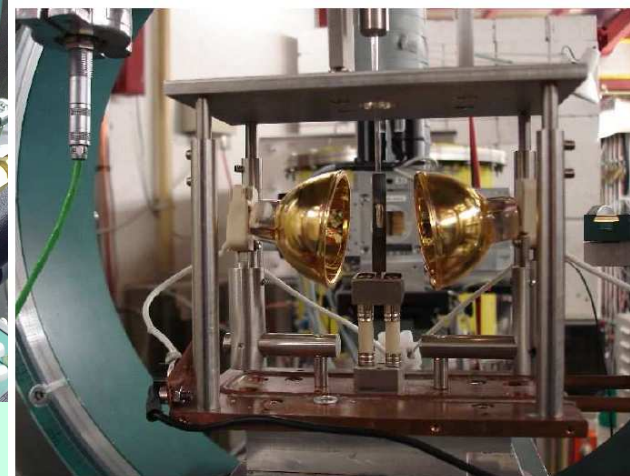
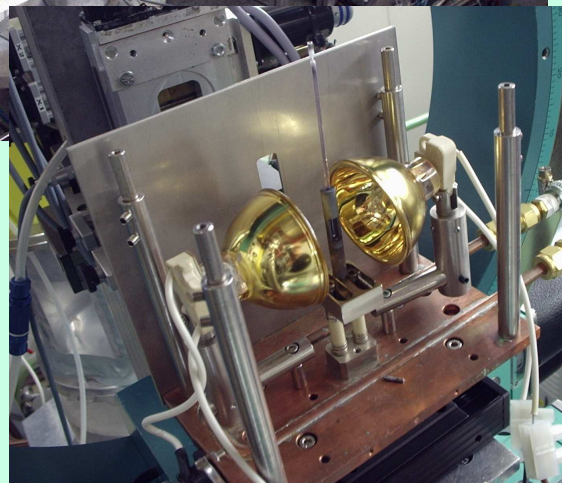
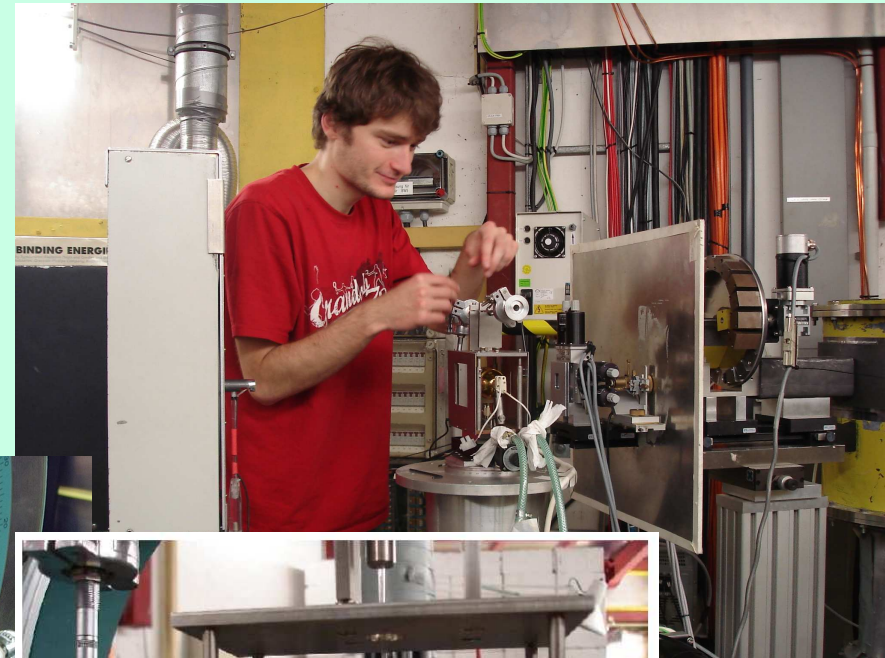
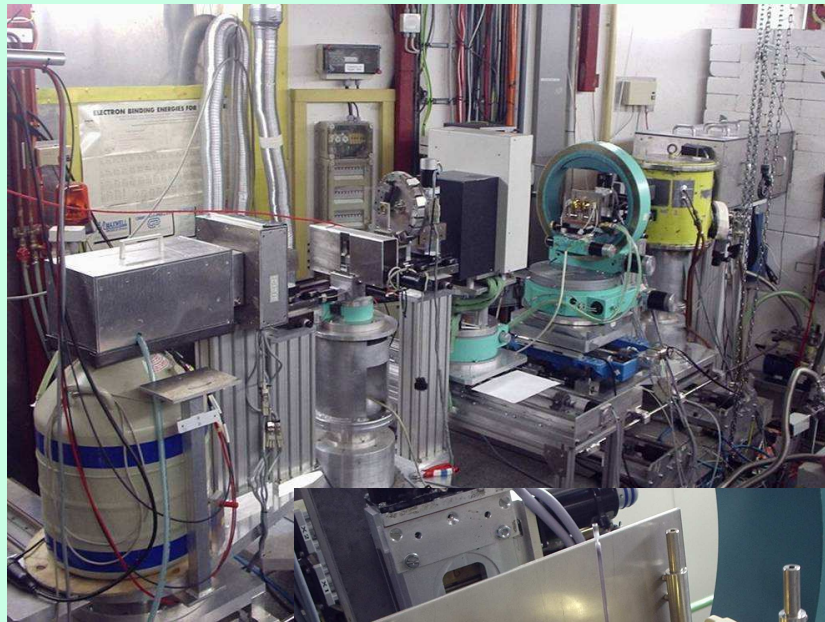


UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH  
Prírodovedecká fakulta

Múdrost' minulosti – poznatky prítomnosti – vzdelanie budúcnosti.



# Experimental station BW5



5 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
[www.science.upjs.sk](http://www.science.upjs.sk)



UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH  
Prírodovedecká fakulta

Múdrost' minulosti – poznatky prítomnosti – vzdelanie budúcnosti.



# Photon energy, wavelength and penetration depth

$$\lambda[\text{\AA}] = \frac{hc}{\varepsilon} = \frac{12.398}{\varepsilon[\text{keV}]}$$

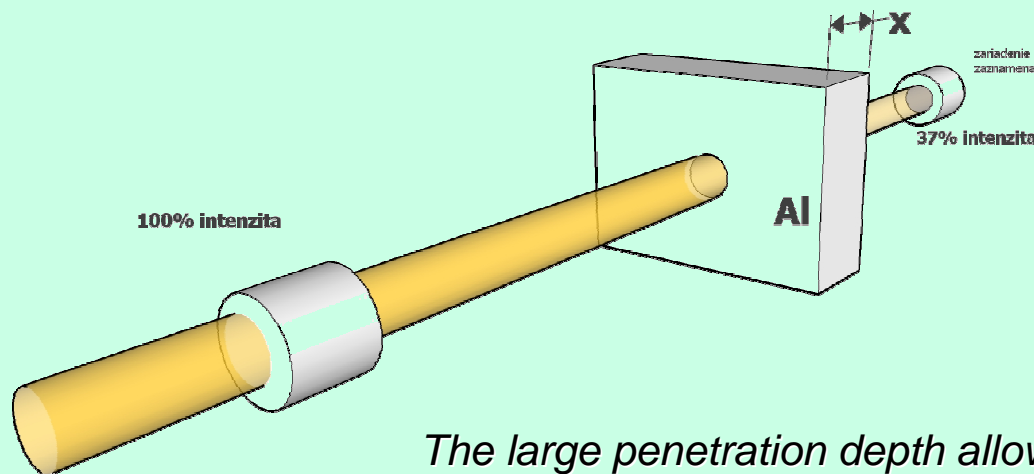
$$\text{\AA} = 10^{-10} \text{ m}$$

$$\text{eV} = 1.602 \times 10^{-19} \text{ J}$$

$$200 \text{ eV} = 62 \text{ \AA} \text{ soft x-rays}$$

$$8.05 \text{ keV} = 1.54 \text{ \AA} \text{ standard x-ray Cu lamp}$$

$$100 \text{ keV} = 0.124 \text{ \AA} \text{ hard x-rays}$$



$$200 \text{ eV} \quad x = 0.1 \text{ }\mu\text{m}$$

$$9 \text{ keV} \quad x = 0.103 \text{ mm}$$

$$100 \text{ keV} \quad x = 2.2 \text{ cm !!!}$$

*The large penetration depth allows the investigation of bulk materials and complex sample environments.*

6 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
www.science.upjs.sk



UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH

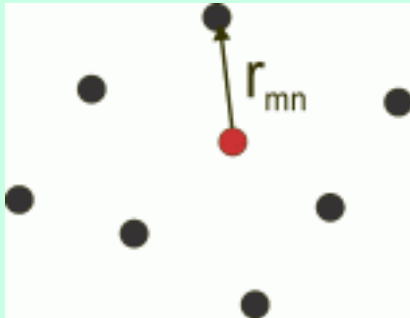
Prírodovedecká fakulta



Múdrost' minulosti – poznatky prítomnosti – vzdelanie budúcnosti.

# Theory of diffraction on disordered materials

The scheme of amorphous alloys



$$I(\mathbf{Q}) = \sum_m^N f_m(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_m} \sum_n^N f_n(\mathbf{Q}) e^{-i\mathbf{Q}\cdot\mathbf{r}_n}$$

$$S(Q) \equiv \frac{I(Q) / N - f^2(Q)}{f^2(Q)} = 1 + \int_0^\infty \underbrace{4\pi r [\rho(r) - \rho_0]}_{D(r)} \frac{\sin(Qr)}{Q} dr$$

where  $\rho(r)$  and  $\rho_0$  are the local and average atomic number densities.  $D(r)$  – the reduced pair distribution function

*Fourier transformation*

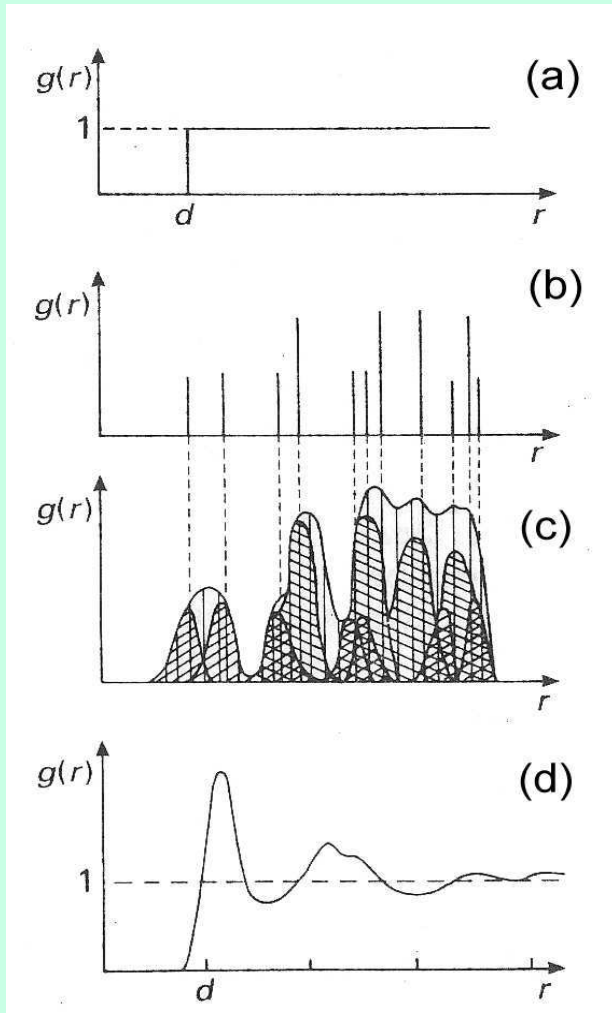
$$S(Q) = \int_0^\infty D(r) \frac{\sin(Qr)}{Q} dr$$

$$D(r) = \frac{2}{\pi} \int_0^\infty Q [S(Q) - 1] \sin(Qr) dQ$$

We are able **directly** to perform the real space analysis (in the space of interatomic distances)



# Pair distribution functions



gas

ideal  
crystal

real  
crystal

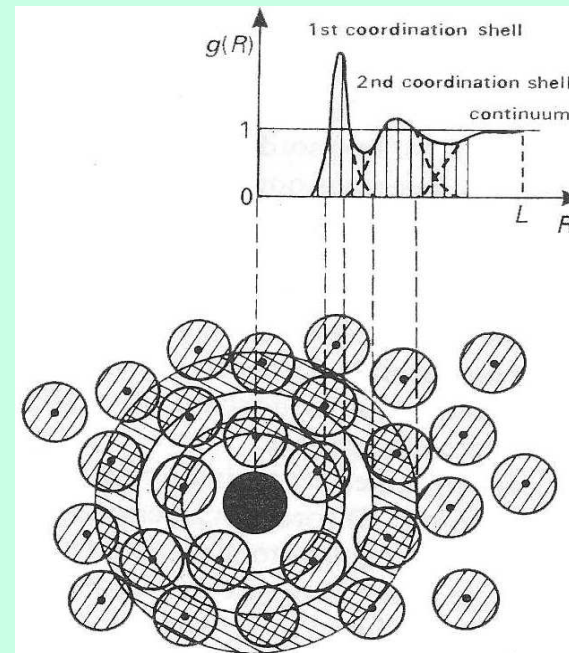
amorphous  
alloy

The reduced distribution function  $D(r)$

$$D(r) = 4\pi r[\rho(r) - \rho_0]$$

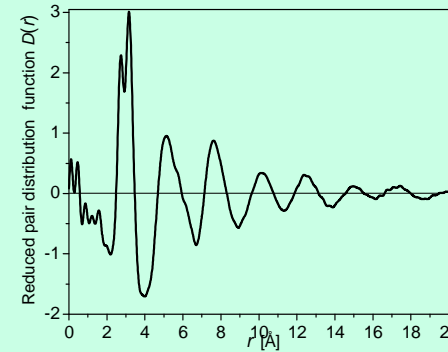
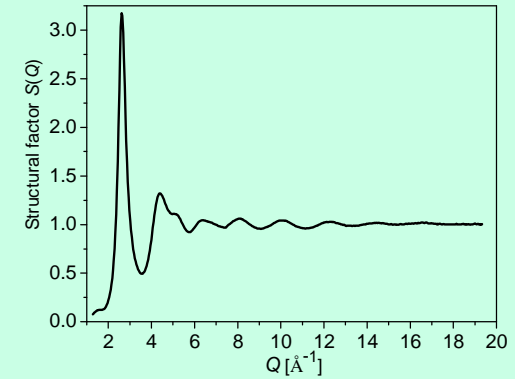
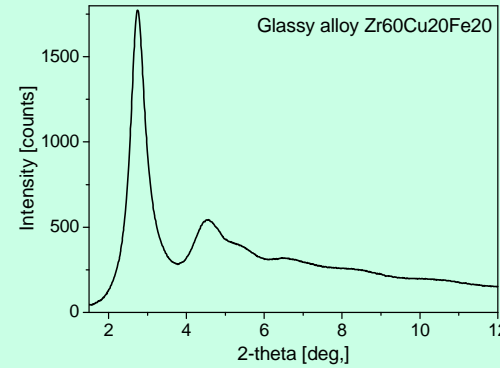
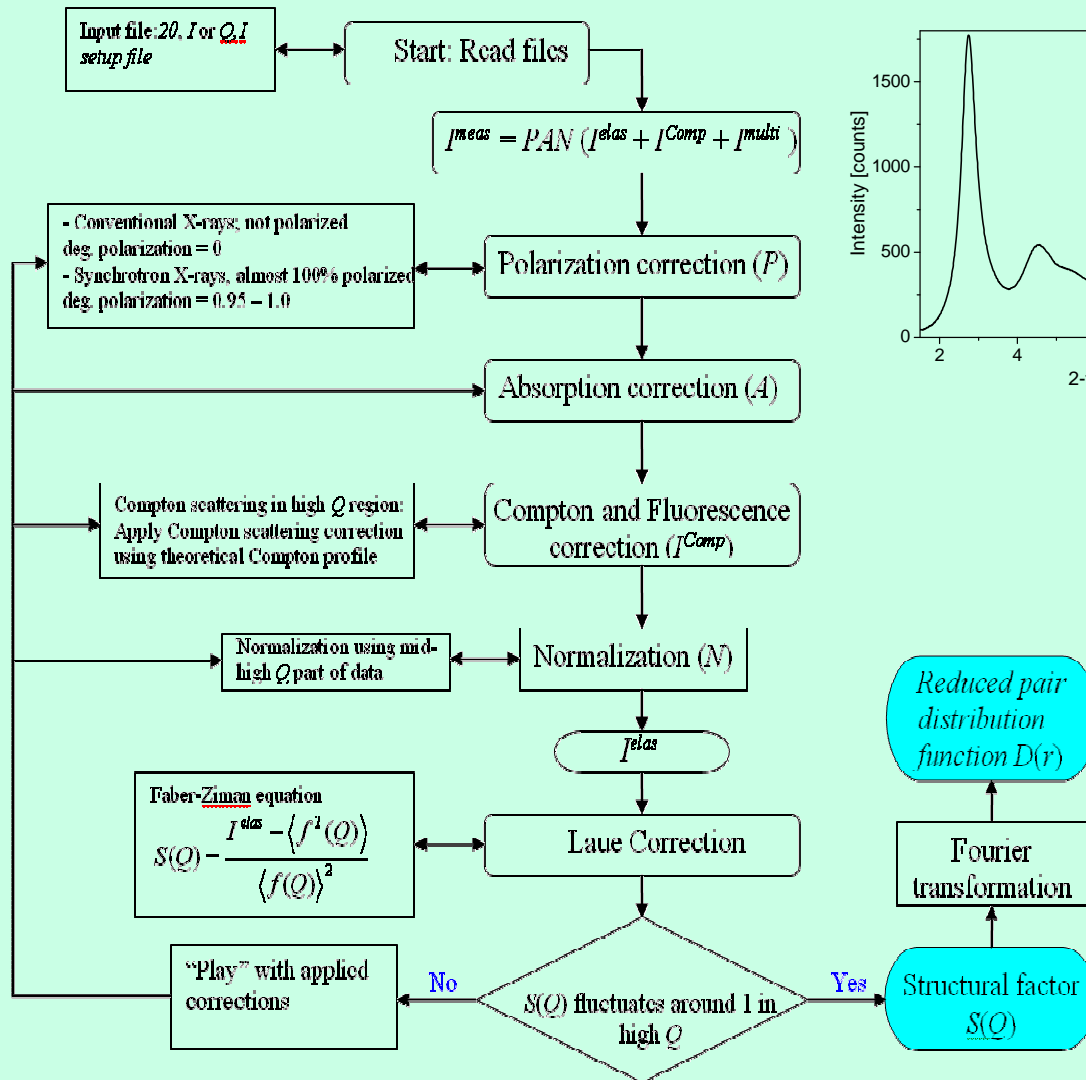
The atomic pair distribution function  $g(r)$

$$g(r) = \rho(r) / \rho_0$$





# The structural factor extraction



Reduced pair distribution function  $D(r)$

Fourier transformation

Structural factor  $S(Q)$

How to do it?

Software PDFGetX2

<http://www.pa.msu.edu/cmp/billinge-group/programs/PDFGetX2/>



# Preprocess a data file

The image shows a multi-step software workflow for preprocessing a data file. The main window is PDFgetX2 v1.0 build 20040722, which is used to open and edit PDF files. A menu path is shown: File -> Preprocess SPEC Format Data -> Get X-Ray PDF. This leads to the EditSPECFormat window, where data file settings are configured: Data Type is 'n x m ascii', Number of lines to skip is '1', Comment identifier is 'Pound', and Delimiter is 'TAB'. The main PDFgetX2 window shows a file named 'Zr70Cu10Pd20\_lvs2T.pdf' with an 'Edit Format' button circled in red. The 'Column & Detector Setup' section is also visible, showing detector configurations. The 'Data Visualization' section includes options for 'Fast Overview', 'Simple Plot View', and 'Raw SPEC'. The 'XY Plot' window displays a graph of 'Col# 2' vs 'Col# 1' with a prominent peak at approximately 8.4990. Red arrows and numbers (1-10) indicate the sequence of actions: 1. Open PDFgetX2, 2. Open EditSPECFormat, 3. Click Edit Format, 4. Select X Column, 5. Select Y Column, 6. Click Plot Data, 7. Click Plot Legend, 8. Click Zoom, 9. Click DeGlitch, 10. Click Center.

10 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
www.science.upjs.sk

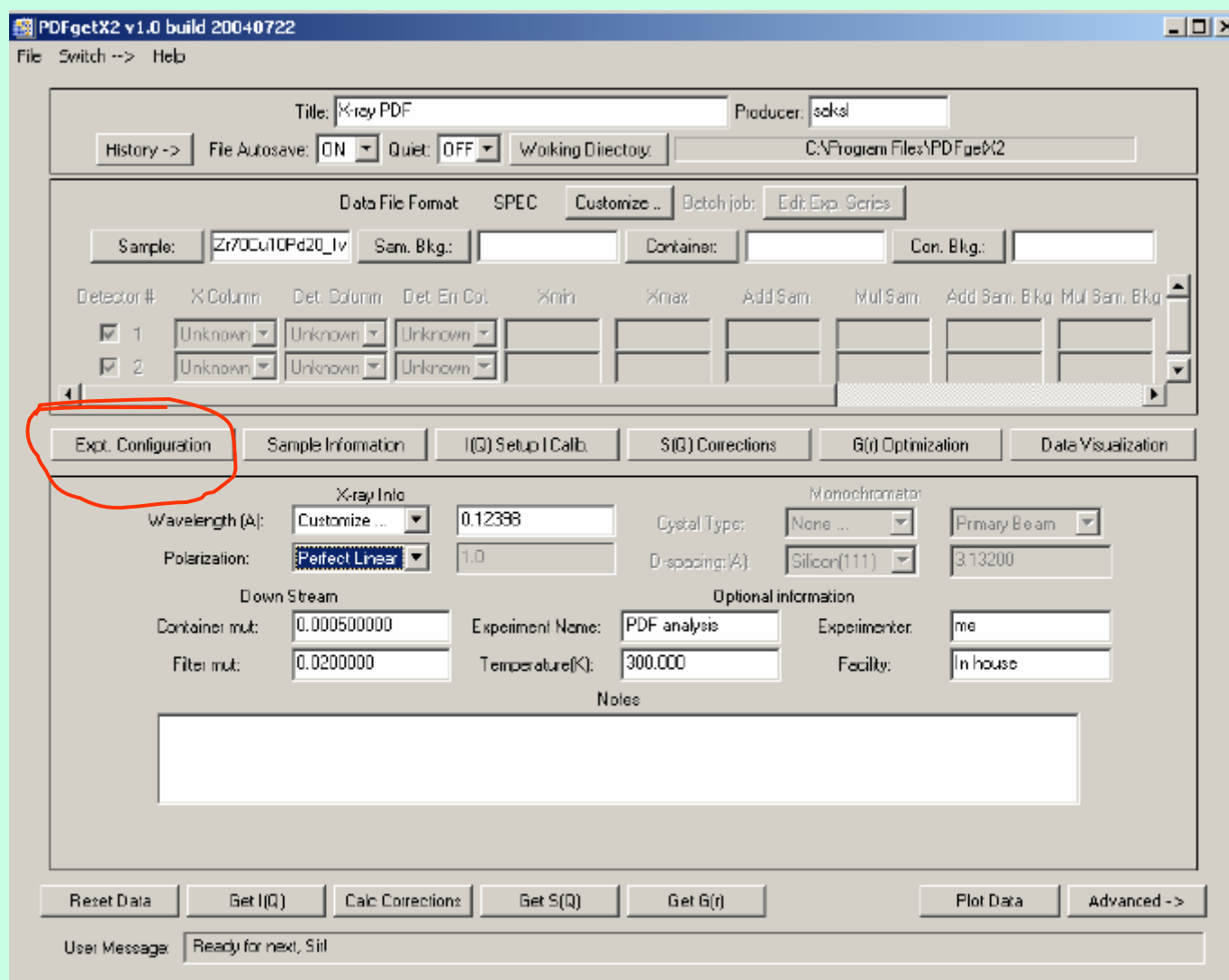


UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH  
Prírodovedecká fakulta

Múdrosť minulosti – poznatky prítomnosti – vzdelanie budúcnosti.



# Setup an exp. configuration



Define wavelength and polarization.

11 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
www.science.upjs.sk



UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH  
Prírodovedecká fakulta

Múdrost' minulosti – poznatky prítomnosti – vzdelanie budúcnosti.



# Setup the sample information

The screenshot displays the PDFgetX2 v1.0 build 20040722 interface. The main window shows the 'Sample Information' tab, which includes fields for Title (X-ray PDF), Producer (saks), and Sample (Zr70Cu10Pd20\_lv). Below these are detector parameters for two detectors, including columns, error models, and various coefficients. A table lists the atoms in the sample:

Symbol	Z	Valence	Fraction	User f1	User f2	User macoef
Zr	40	0.00	0.7000	0.0000	0.0000	0.0010
Cu	29	0.00	0.1000	0.0000	0.0000	0.0010
Pd	46	0.00	0.3000	0.0000	0.0000	0.0010

Optional Info fields include Number Density (0.0485000), Packing Fraction (0.500000), Thickness/Diameter (mm) (2.00000), and Theoretical mut (0.786970). The 'XGetElements' dialog box is open, showing a periodic table with Pd selected. The elements selected are listed as Zr,Cu,Pd.

Define the sample chemical composition, the sample geometry, the number density and other parameters.

Push "Reset Data", "Get I(Q)" and then "Calc Correction" and so the "theoretical mut" will be calculated. The calculated value put into "Attenuation Coef. (mut)".

12 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
www.science.upjs.sk



UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH  
Prírodovedecká fakulta

Múdrost' minulosti – poznatky prítomnosti – vzdelanie budúcnosti.



# I(Q) setup

PDFgetX2 v1.0 build 20040722

File Switch --> Help

Title: X-ray PDF Producer: saksl

History -> File Autosave: ON Quiet: OFF Working Directory: C:\Program Files\PDFgetX2

Data File Format: SPEC Customize... Batch job: Edit Exp. Series

Sample: Zr70Cu10Pd20\_lv Sam. Bkg.: Container: Con. Bkg.:

Detector #	X Column	Det. Column	Det. Err Col.	Xmin	Xmax	Add Sam.	Mul Sam.	Add Sam. Bkg	Mul Sam. Bkg
<input checked="" type="checkbox"/> 1	Col#_1	Col#_2	Dummy	0.00692296	27.9064	0.000000	1.00000	0.000000	1.00000
<input checked="" type="checkbox"/> 2	Unknown	Unknown	Unknown						

Expt. Configuration Sample Information **I(Q) Setup | Calib.** S(Q) Corrections G(r) Optimization Data Visualization

X Column Format: 2 Theta (degree)

Flat Plate Filter Corr.  Effective Absorption Corr.

Sample  Sample Bkg.

To?  Sample Bkg. To?  Container Bkg.

Container  Container

Container Bkg.

Reset Negative Value to: -1.00000

Det. Energy Dependence

X axis: Wavelength

Function Type: Linear

Value @ Elastic: 1.00000

Value @ Fluores: 1.80000

Quadra Scale: 0.000000

Spline Scale: 0.000000

Table File:

Det. Transmission Coef.

X axis: Wavelength

Function Type: Linear

Value @ Elastic: 0.950000

Value @ Fluores: 0.600000

Quadra Scale: 0.000000

Spline Scale: 0.000000

Table File:

Reset Data Get I(Q) Calc Corrections Get S(Q) Get G(r) Plot Data Advanced ->

User Message: [Mon Jun 19 09:41:08 2006] Start to calculate corrections ... successfully finished!

Choose a correct a  
X Coumn Format

13 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
www.science.upjs.sk



UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH

Prírodovedecká fakulta

Múdrosť minulosti – poznatky prítomnosti – vzdelanie budúcnosti.



# Setup $S(Q)$ corrections

PDFgetX2 v1.0 build 20040722

File Switch --> Help

Title: X-ray PDF Producer: saks1

History -> File Autosave: ON Quiet: OFF Working Directory: C:\Program Files\PDFgetX2

Data File Format: SPEC Customize... Batch job: Edit Exp. Series

Sample: Zr70Cu10Pd20\_lv Sam. Bkg.: Container: Con. Bkg.:

Detector #	X Column	Det. Column	Det. Err Col.	Xmin	Xmax	Add Sam.	Mul Sam.	Add Sam. Bkg	Mul Sam. Bkg
<input checked="" type="checkbox"/> 1	Col#_1	Col#_2	Dummy	1.20000	19.0000	0.000000	1.00000	0.000000	1.00000
<input checked="" type="checkbox"/> 2	Unknown	Unknown	Unknown						

Expt. Configuration Sample Information I(Q) Setup | Calib. **S(Q) Corrections** G(r) Optimization Data Visualization

Method:  Generic  I(Q) Simu. SetUp: Elastic

Sample Self-Absorption  Compton Scattering

Multiple Scattering (2nd only) profile: emperical form

Oblique Incidence Transmissoin Coeff.: 0.980000

Fluorescence Type: Constant Scale: 430.0000

X-ray Polarization

Laue Diffuse Scattering

Weighting Function Type: <math>\langle \text{asf} \rangle^2</math>

Qstart: 3.00000 Width: 100 Cycles: 600

Edit S(Q) w/: Const. + 0.00000 \* 1.00000

Qstart: 3.00000 Width: 100 Cycles: 600

Smoothing Qmin: 12.0000 Width: 9

Damp F(Q) Type: Gaussian Width (Å) 23.00

Interpolate Qmin to 0.0 Linear

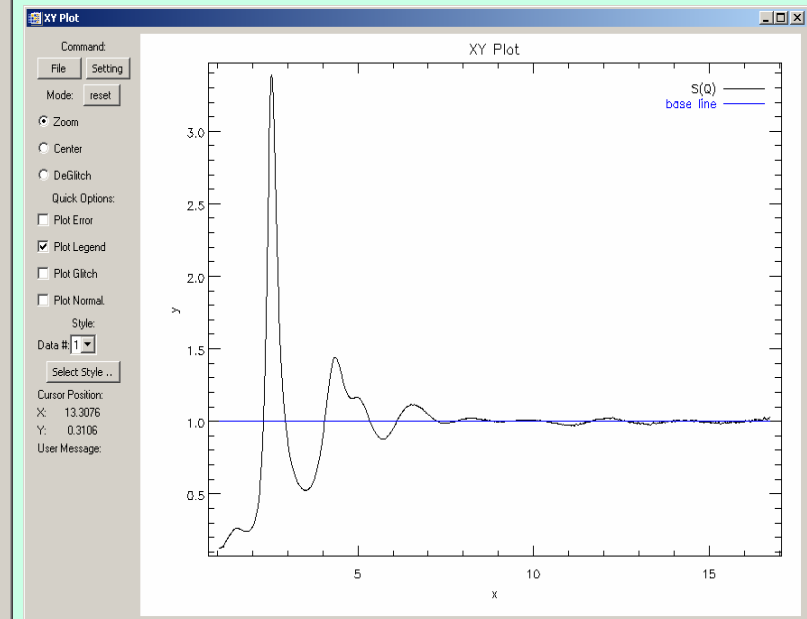
Auto Scale manual: 0.172768 High Q Range: 60 % calc: 0.17276858

Reset Data Get I(Q) Calc Corrections Get S(Q) Get G(r) Plot Data Advanced ->

User Message: [Mon Jun 19 10:04:16 2006] Start to obtain S(q) ... successfully completed!

Apply all necessary correction in order that  $S(Q)$  oscillates around 1.

Push "Get S(Q)"



14 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
www.science.upjs.sk



UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH

Prírodovedecká fakulta

Múdrost' minulosti – poznatky prítomnosti – vzdelanie budúcnosti.



# Data visualization

PDFgetX2 v1.0 build 20050123

File Switch -> Help

History -> Title: X-ray PDF Producer: Preuser

Working Directory: C:\Program Files\PDFgetX2 File Autosave: Quiet

Data File Format: SPEC Customize... Batch job: Edit Exp. Series

Sample: Sam. Bkg.: Container: Con. Bkg.:

Detector #: X Column Det. Column Det. Err. Col. Xmin Xmax Add Sam. Mul Sam. Add Sam. Bkg. Mul Sam. Bkg.

Expt. Configuration Sample Information I(Q) Setup | Calib. S(Q) Corrections G(r) Optimization **Data Visualization**

Data Type:
 

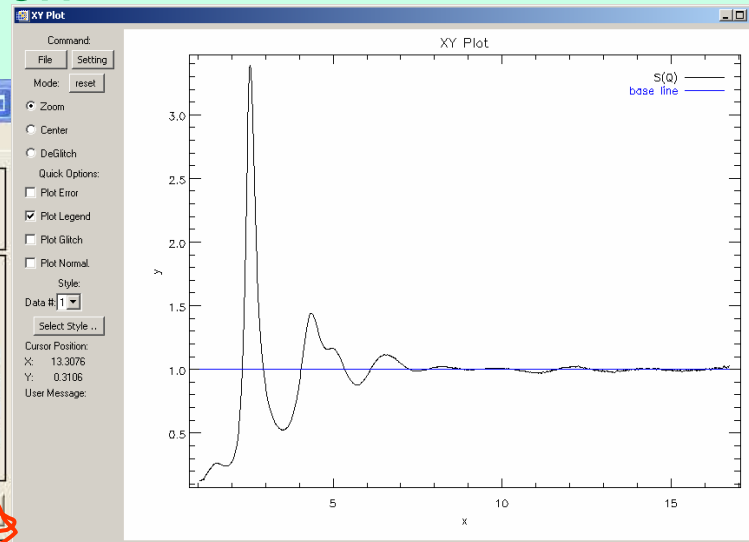
- Raw Data
- I(Q) Corrections
- I(Q)
- I(Q) Simulations
- S(Q) Corrections
- S(Q) to F(Q)**
- G(r) Opt.
- G(r)
- Calibrations

Corrections:
 

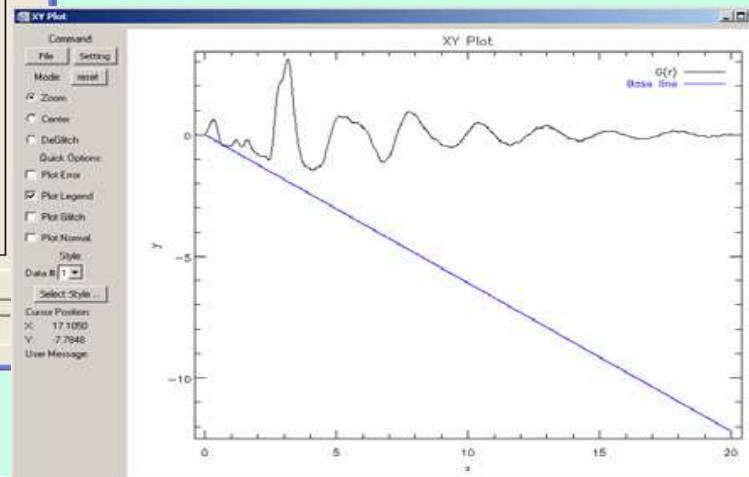
- Editing
- Filter Corr.
- Absorp. Corr.
- Bkg. Subtr.
- Con. Subtr.
- Init. Int.
- Samp. Absorp.
- Multi-Scat.
- X-ray Polar.
- Oblincident.
- Energy Dep.
- B-D Recoil.
- Ruland Win.
- Simult. Int.
- Simult. I(Q)
- Self Absorp.
- Multi-Scat.
- Oblincident.
- Fluores.
- X-ray Polar.
- Compton Scat.
- Ruland Win.
- B-D Recoil.
- Det. Effici.
- Laue Diffuse
- ASF Weighted
- User Edit
- Smooth BoxCar
- S(Q)**
- Damping Func.
- Qmin Interp.
- F(Q)
- F(Q)
- G(r)
- Atom ASFs
- Comptons
- Det. T\_Coeff.
- Energy Dep.

Reset Data Get I(Q) Calc Corrections Get S(Q) Get G(r) Plot Data Advanced ->

User Message: Ready for next, Sir!



Push "Get G(r)"



15 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
www.science.upjs.sk



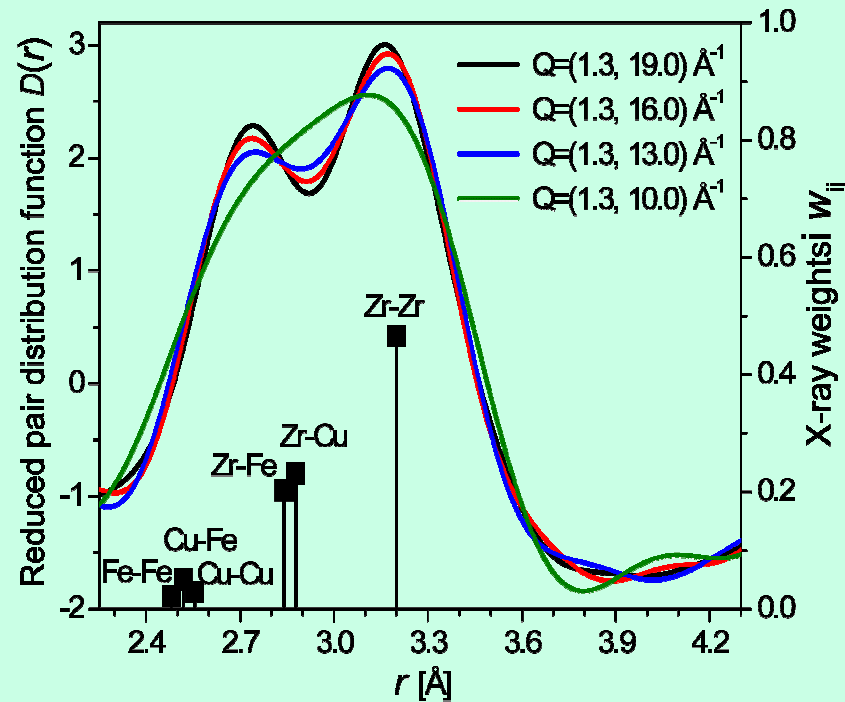
UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH  
Prírodovedecká fakulta

Múdrosť minulosti – poznatky prítomnosti – vzdelanie budúcnosti.



## One example – is the high Q needed?

First coordination shell of  $D(r)$  of the  $Zr_{60}Fe_{20}Cu_{20}$  glassy alloy.



Atomic pairs	Interatomic bond lengths [Å]	X-ray weights $w_{ij}$
Zr-Zr	3.200	0.4660
Zr-Cu	2.878	0.2313
Zr-Fe	2.841	0.2020
Cu-Fe	2.519	0.0501
Cu-Cu	2.556	0.0287
Fe-Fe	2.482	0.0219

We need the  $Q$  vector as high as possible in order to improve the resolution  $\Delta r$  in the real space.

$$\Delta r = (Q_{\max} - Q_{\min}) / \pi$$

Shortening of interatomic Zr-Fe and Zr-Cu distances about 3.5 % is observed.

16 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
www.science.upjs.sk



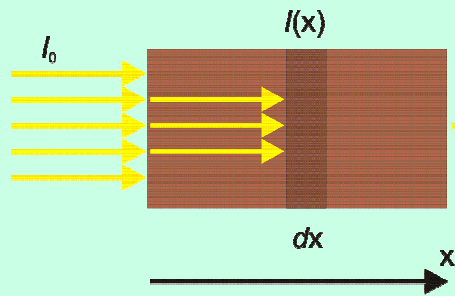
UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH  
Prírodovedecká fakulta



Múdrost' minulosti – poznatky prítomnosti – vzdelanie budúcnosti.

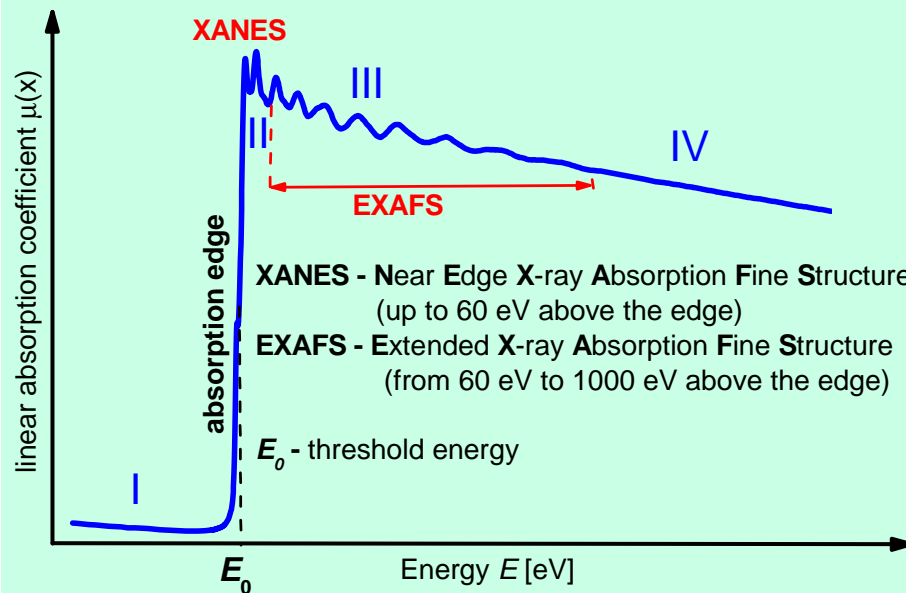


# X-ray absorption



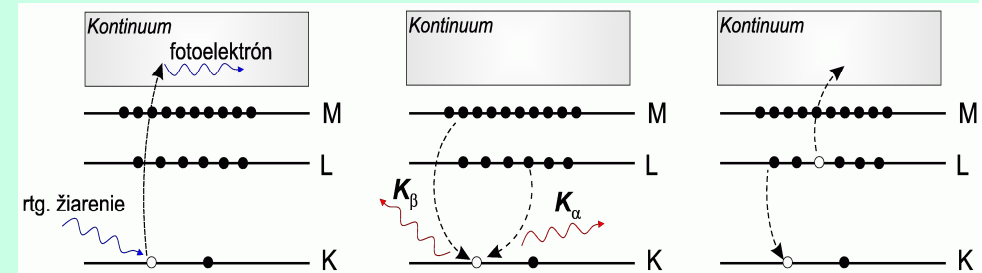
$$I = I_0 e^{-\mu(E)x}$$

$$\mu(E) \approx \frac{\rho Z^4}{E^3}$$



## Fermi golden rule

$$\mu(E) \propto \sum_f \left| \langle \psi_f | \hat{\mathbf{e}} \cdot \mathbf{r} | \psi_i \rangle \right|^2 \delta(E_f - E_i - \hbar\omega)$$



emission of a photoelectron

characteristic x-rays are emitted

Auger's electrons are produced

17 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
www.science.upjs.sk



UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH

Prírodovedecká fakulta

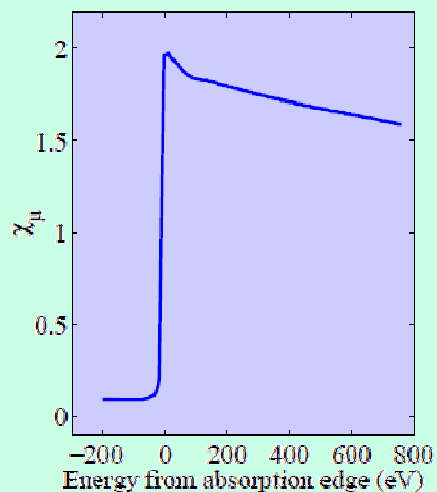
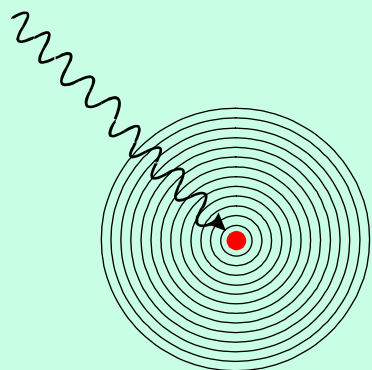


Múdrost' minulosti – poznatky prítomnosti – vzdelanie budúcnosti.

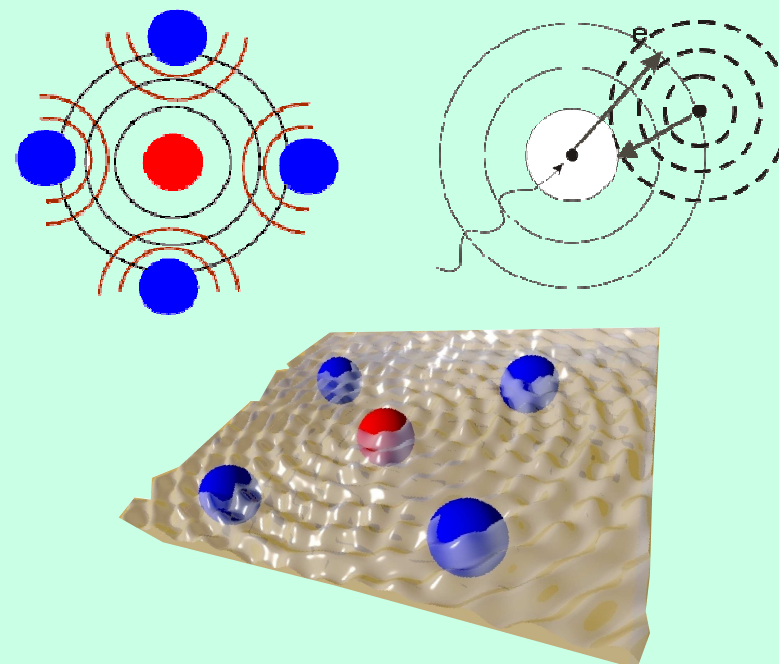
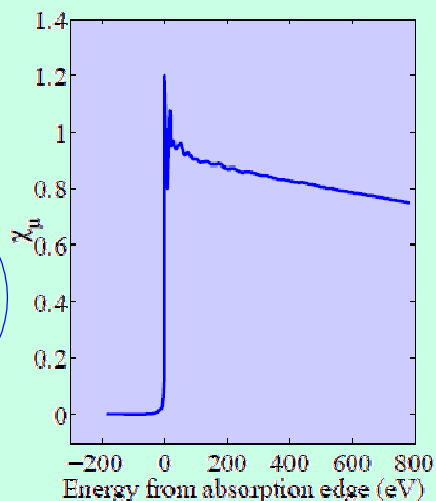
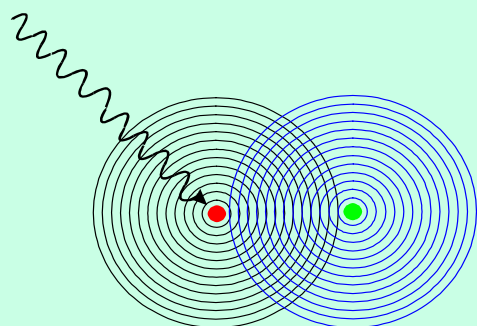
# X-ray absorption fine structure signal (XAFS)

## Explanation

XAFS of one atom  
(inert gases)



XAFS of two atoms



XAFS is the result of interference effects of outgoing and backscattered photoelectrons.

Oscillations of  $\mu(E)$  are a unique fingerprint of a local atomic structure around an absorbing atom.

18 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
www.science.upjs.sk



UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH

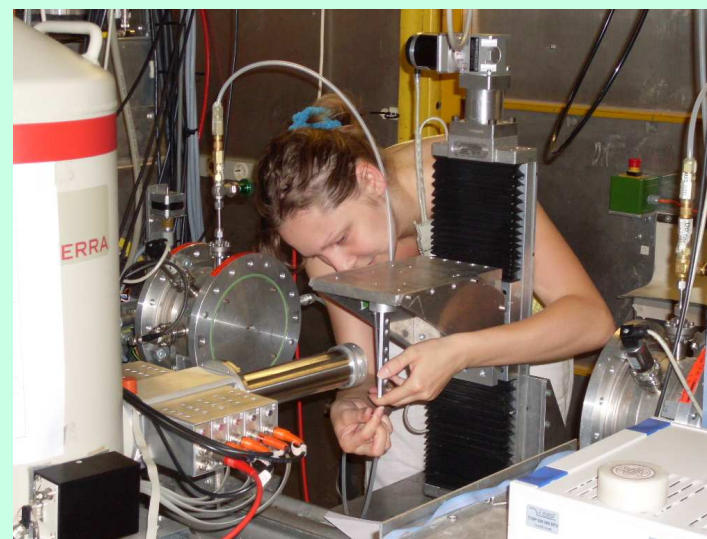
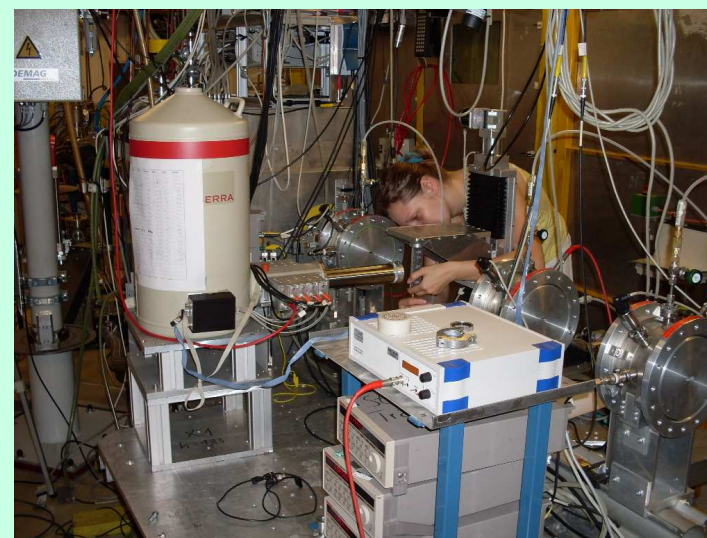
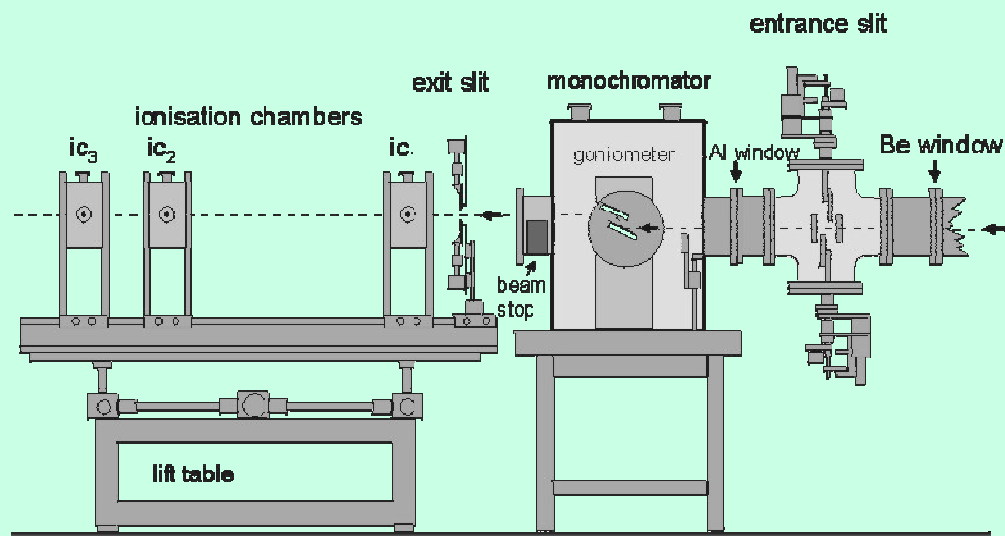
Prírodovedecká fakulta



Múdrost' minulosti – poznatky prítomnosti – vzdelanie budúcnosti.

# Experimental realization

## Setup of the X1 experiment



### Modes of realization

Transmission mode: the most preferable, easiest for realization and data correction

Fluorescence mode: characteristic x-rays are detected

Total electron yield mode: electrons are detected

19 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
www.science.upjs.sk



UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH

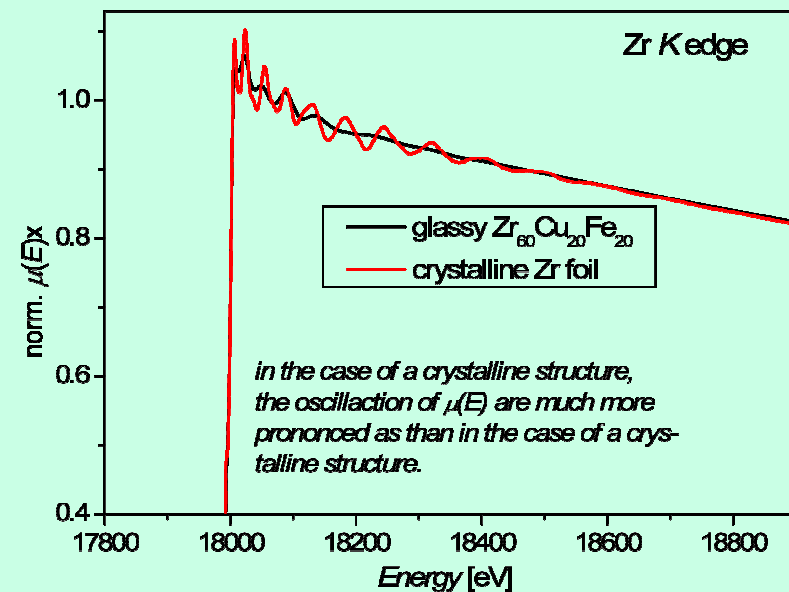
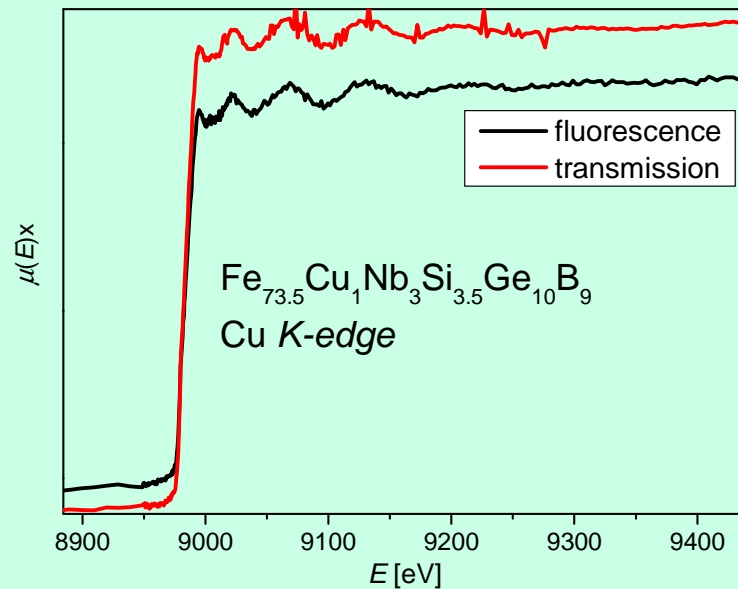
Prírodovedecká fakulta



Múdrost' minulosti – poznatky prítomnosti – vzdelanie budúcnosti.

# Experimental realization – practical aspects

Transmission mode – a sample must be homogeneous with constant thickness, absorption  $\mu(E)x < 2.6$ , not too low concentration of absorbing atoms



Example for a  $\text{Fe}_{73.5}\text{Cu}_1\text{Nb}_3\text{Si}_{3.5}\text{Ge}_{10}\text{B}_9$  ribbon:

absorption  $\mu(E)x = 2.0$

Fe K-edge:  $x = 8.5 \mu\text{m}$

Cu K-edge:  $x = 15.2 \mu\text{m}$

Nb K-edge:  $x = 85 \mu\text{m}$

Ge K-edge:  $x = 21.9 \mu\text{m}$

low absorbing element concentration results in spikes and strong background tail contribution

20 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
www.science.upjs.sk



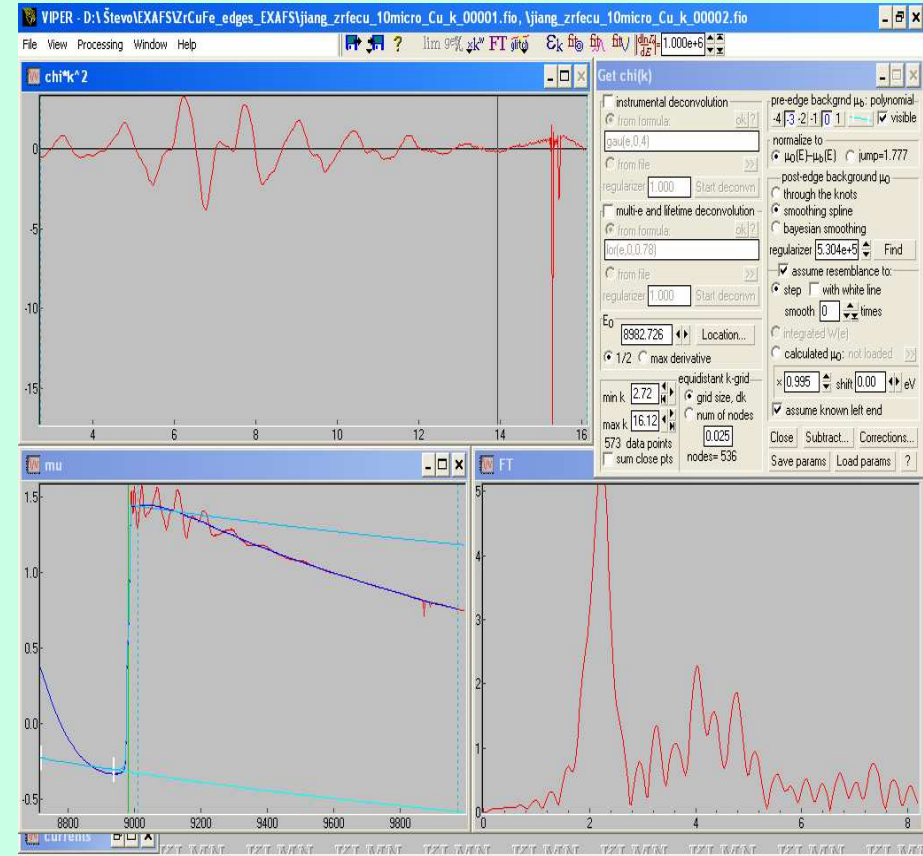
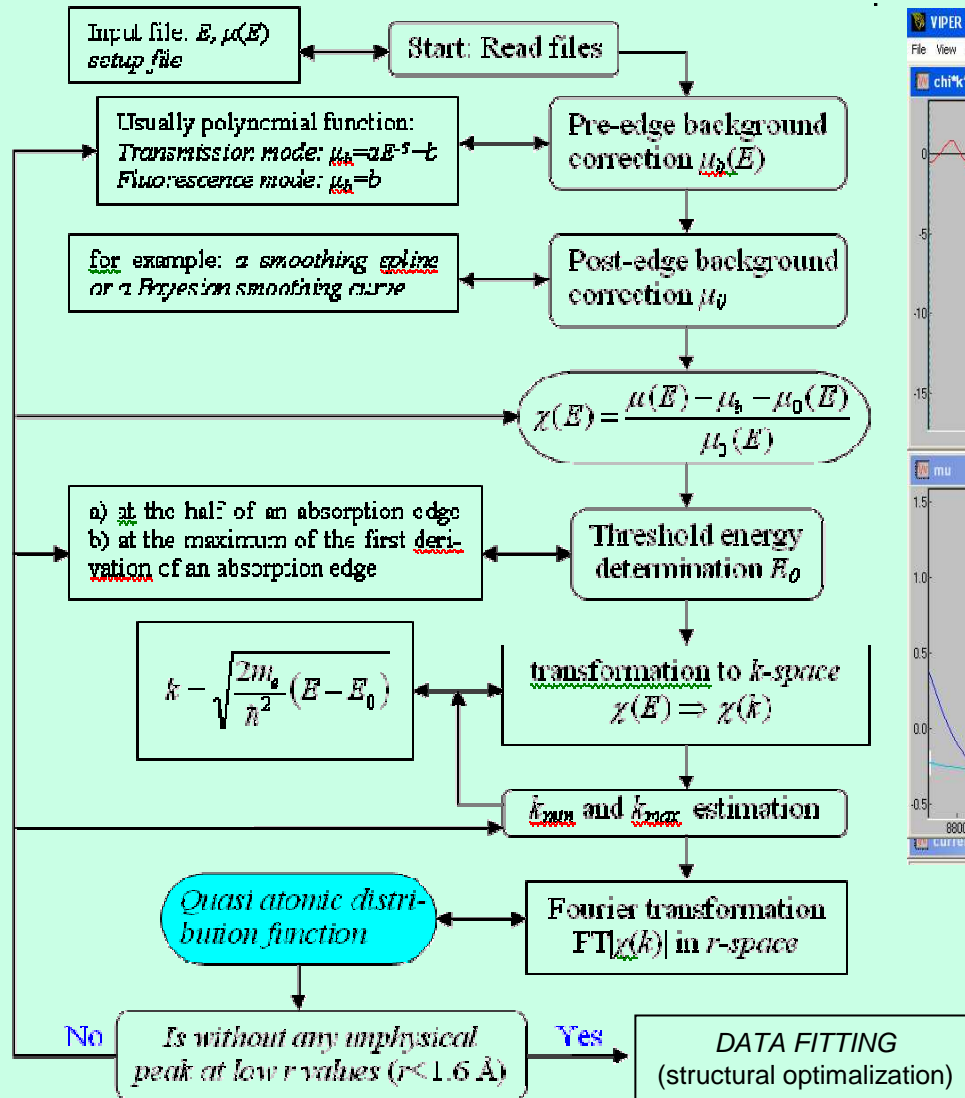
UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH

Prírodovedecká fakulta



Múdrost' minulosti – poznatky prítomnosti – vzdelanie budúcnosti.

# Data processing



## Software VIPER

<http://www.cells.es/Beamlines/CLAESS/software/viper.html>

21 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
[www.science.upjs.sk](http://www.science.upjs.sk)



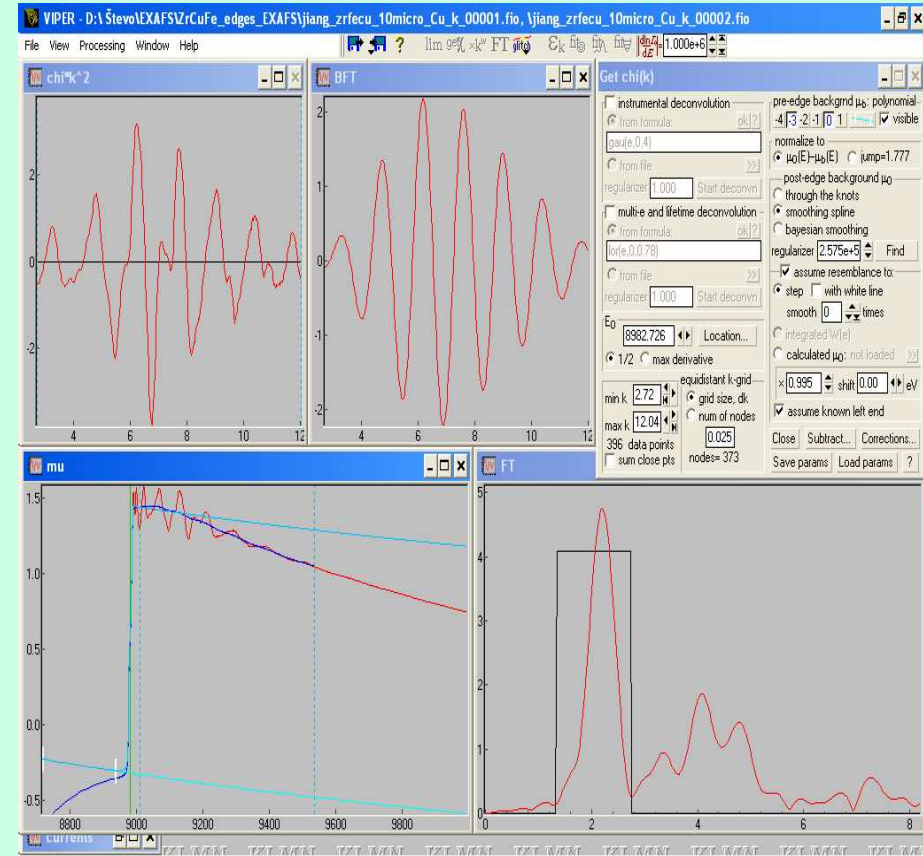
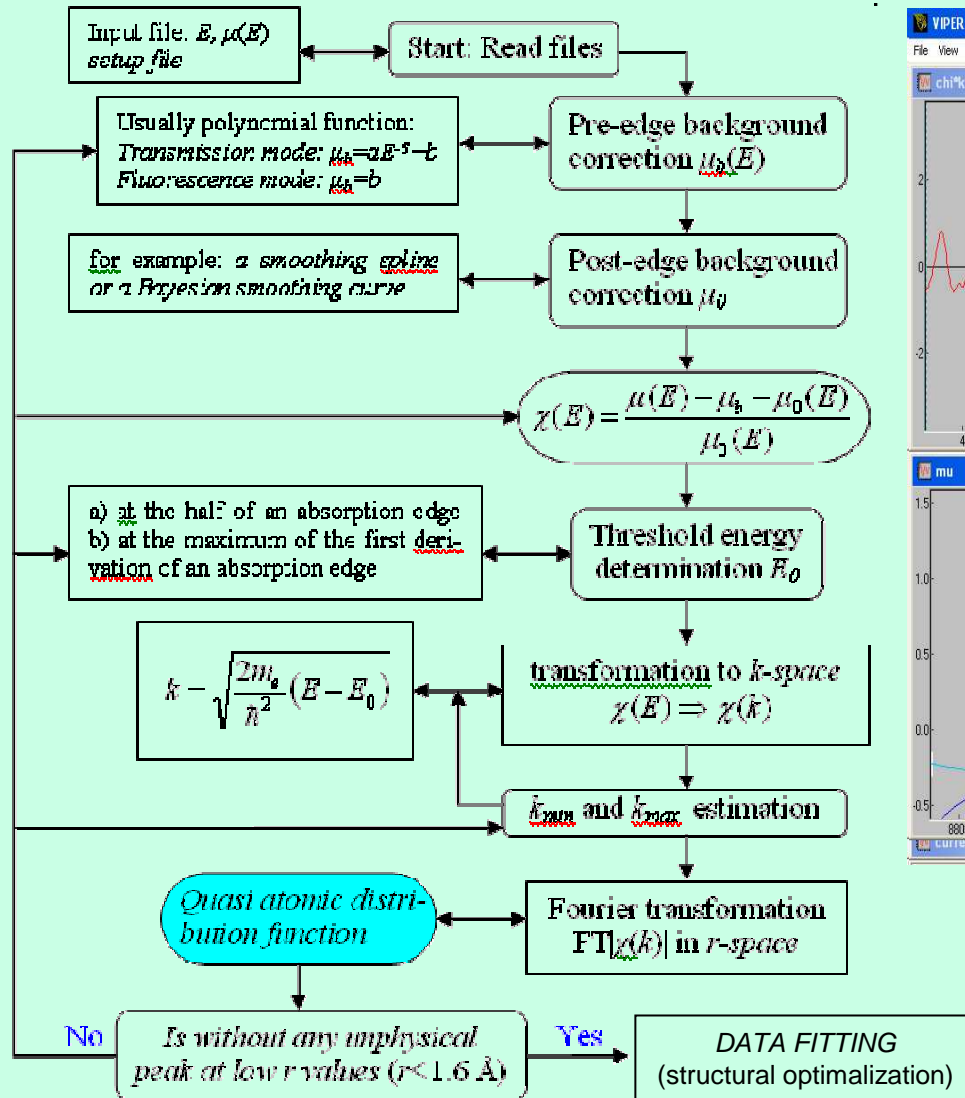
UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH

Prírodovedecká fakulta



Múdrost' minulosti – poznatky prítomnosti – vzdelanie budúcnosti.

# Data processing



22 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
www.science.upjs.sk



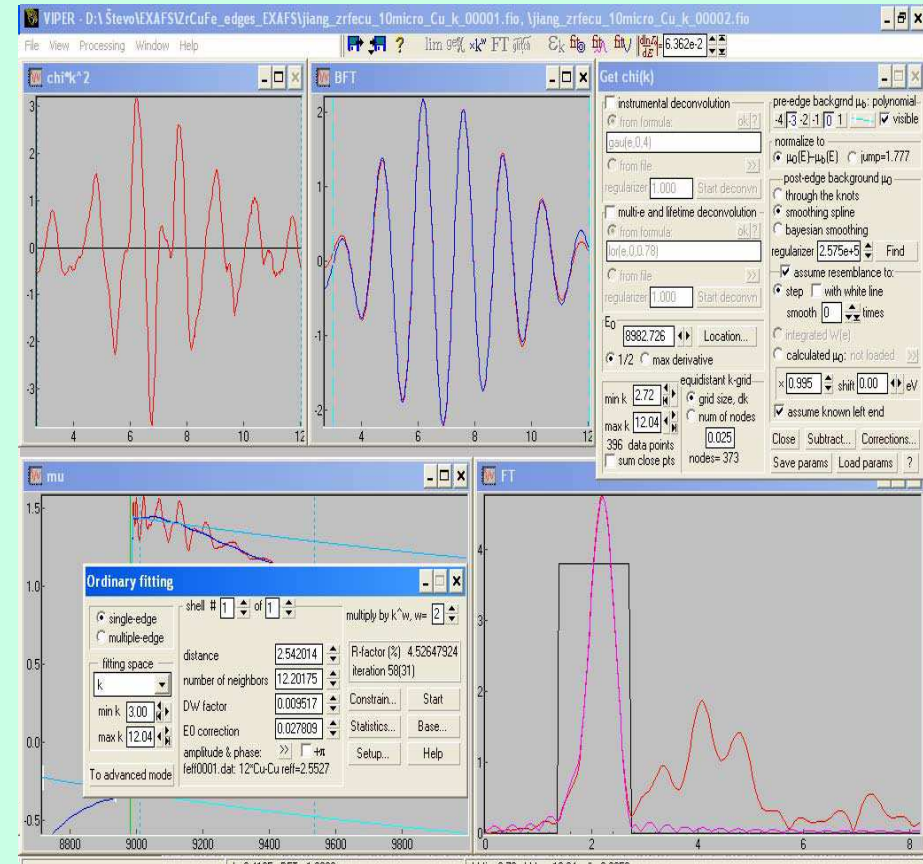
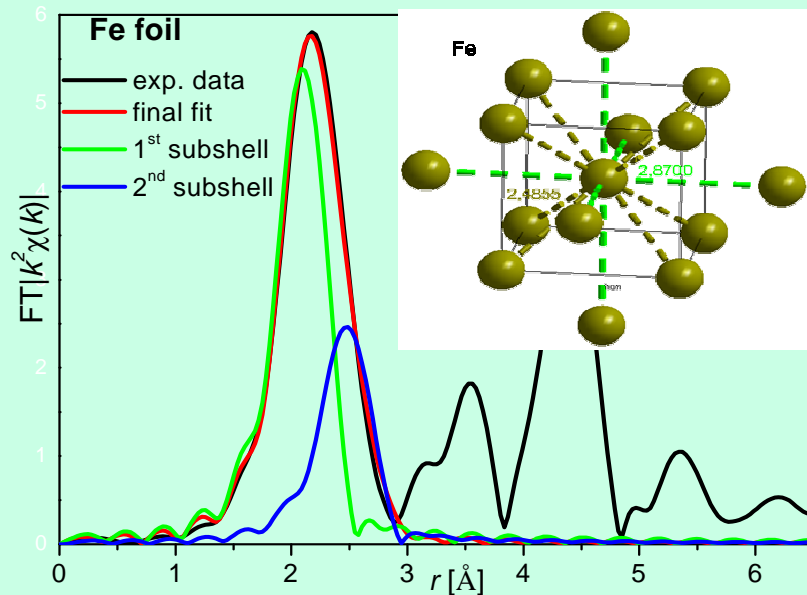
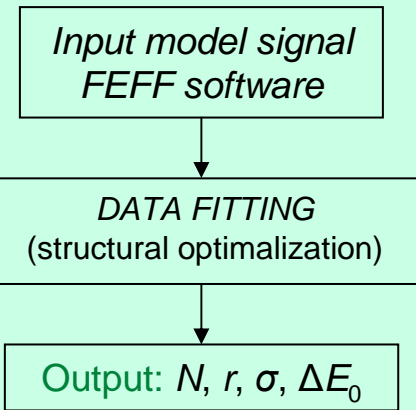
UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH

Prírodovedecká fakulta



Múdrost' minulosti – poznatky prítomnosti – vzdelanie budúcnosti.

# Data processing



23 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
www.science.upjs.sk

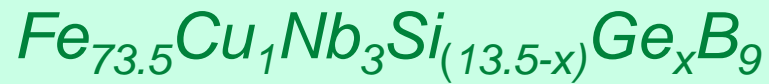


UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH  
Prírodovedecká fakulta

Múdrosť minulosti – poznatky prítomnosti – vzdelanie budúcnosti.

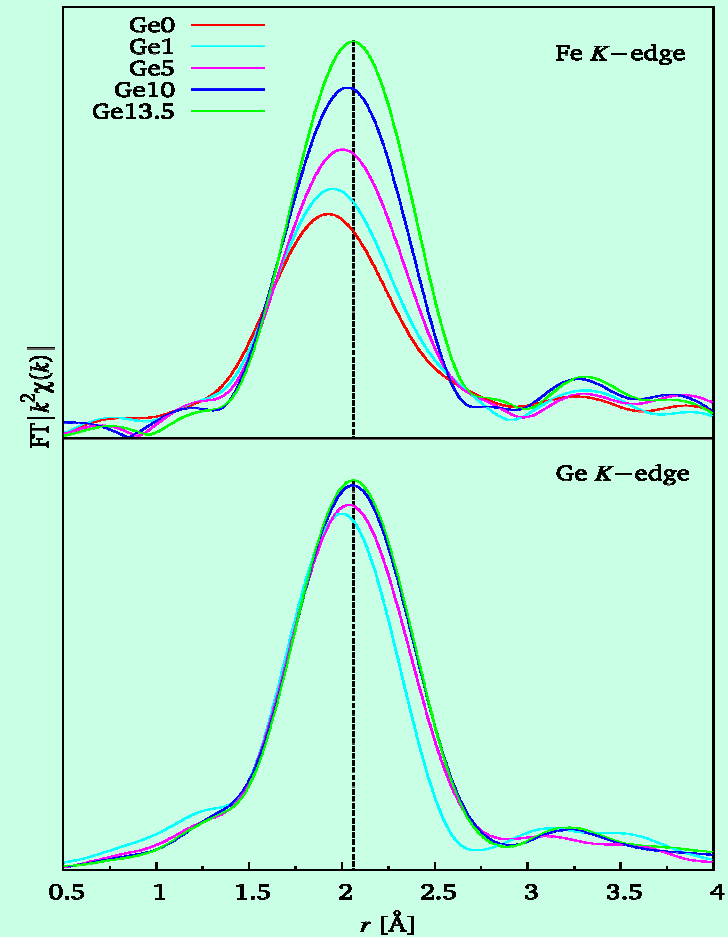
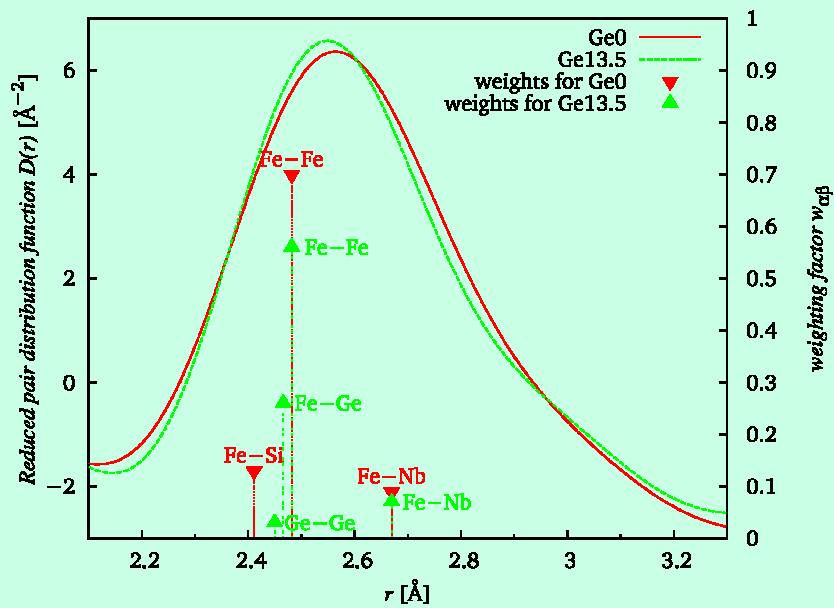


# One example



## EXAFS – real space

## XRD – real space



24 18.2.2011

PF UPJŠ v Košiciach  
 Moyzesova 16, 041 54 Košice  
 www.science.upjs.sk



UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH

Prírodovedecká fakulta



Múdrosť minulosti – poznatky prítomnosti – vzdelanie budúcnosti.

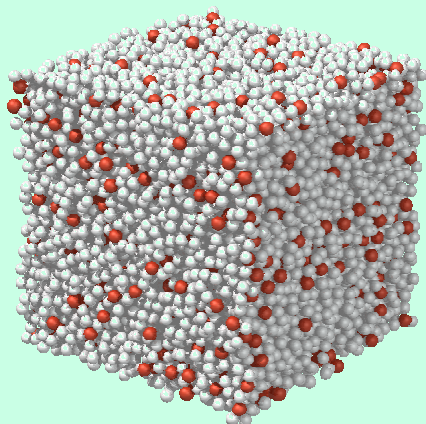


# Principle of RMC modeling

The aim is to minimize difference between functions obtained from model and experiment

$$\psi^2 = \frac{1}{\delta} \sum_{i=1}^m [\zeta^{\text{exp}} - \zeta^{\text{RMC}}]^2$$

Box of ~ 10 000 atoms



with constrains:

- minimum interatomic distances
- atomic density

## How???

### 1. Move:

One particle is moved randomly taking into account applied constraints.

### 2. Acceptance of the move:

First the experiment-model difference is calculated

If  $\psi^2_{n+1} < \psi^2_n$  the move is always accepted.

If  $\psi^2_{n+1} > \psi^2_n$  the move is accepted with the probability  $\exp[-(\psi^2_{n+1} - \psi^2_n)/2]$

### 3. Settling:

Everything is repeated until  $\psi^2$  begins to oscillate around a constant value.

Experimental data:

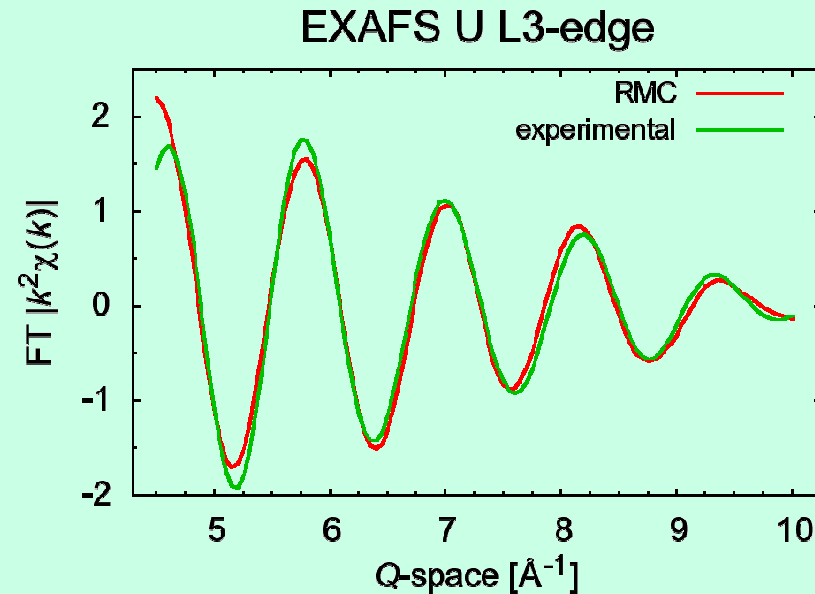
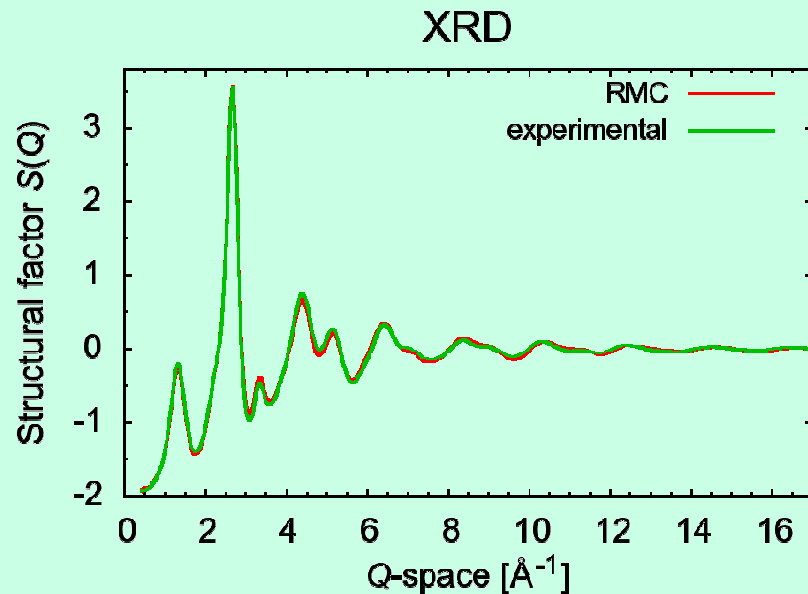
- **XRD**, ND, ED
- **EXAFS**
- SAXS, SANX

### Result:

*We have an 3D structural model which is consistent with experimental data.*



# One example: RMC modelling of a binary $\text{Al}_{92}\text{U}_8$ glassy alloy



Nice match is obtained between experimental data and model data produced on the base of Reverse Monte Carlo simulation



We can perform analysis of the produced 3D structural model.

26 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
www.science.upjs.sk



UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH

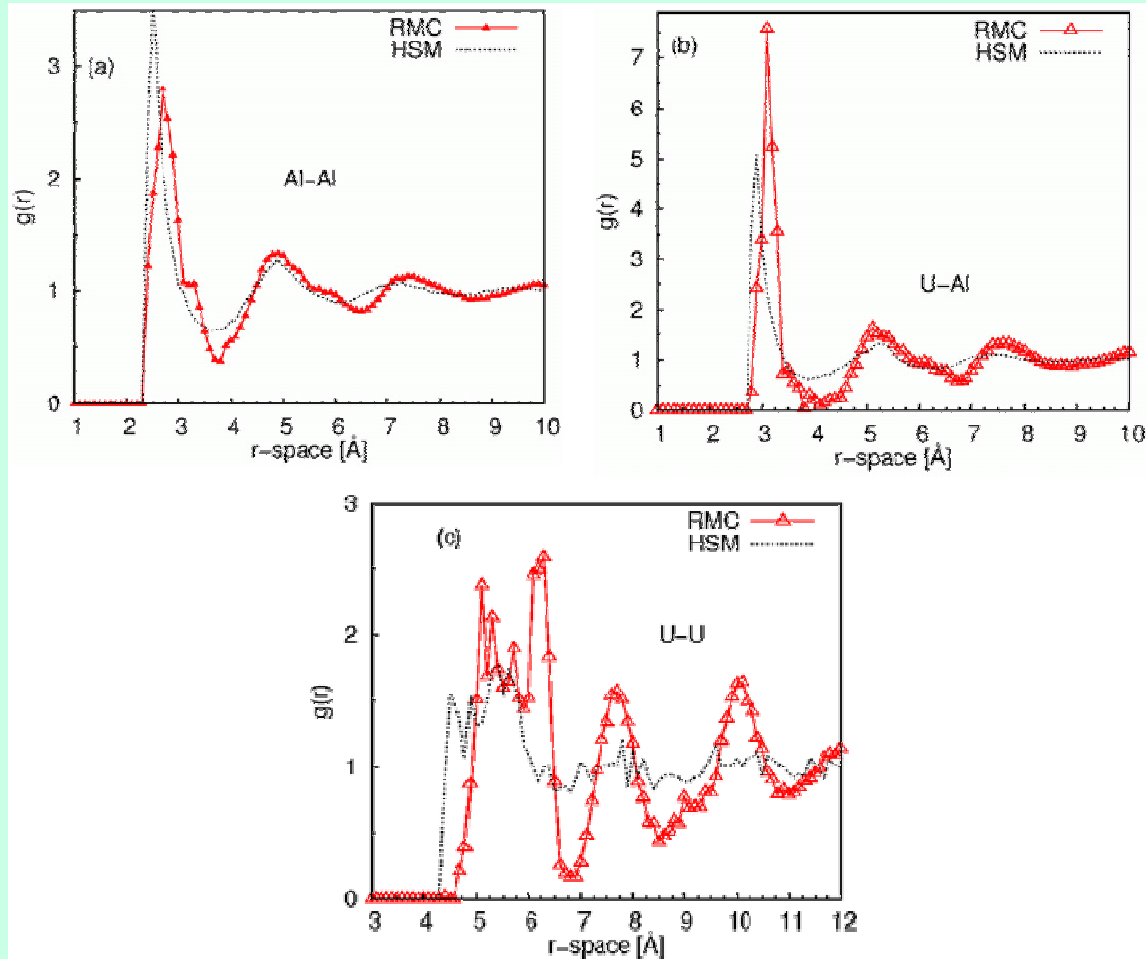
Prírodovedecká fakulta



Múdrost' minulosti – poznatky prítomnosti – vzdelanie budúcnosti.

# RMC modeling

Partial atomic pair distribution functions can be directly calculated !!!



27 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
www.science.upjs.sk



UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH

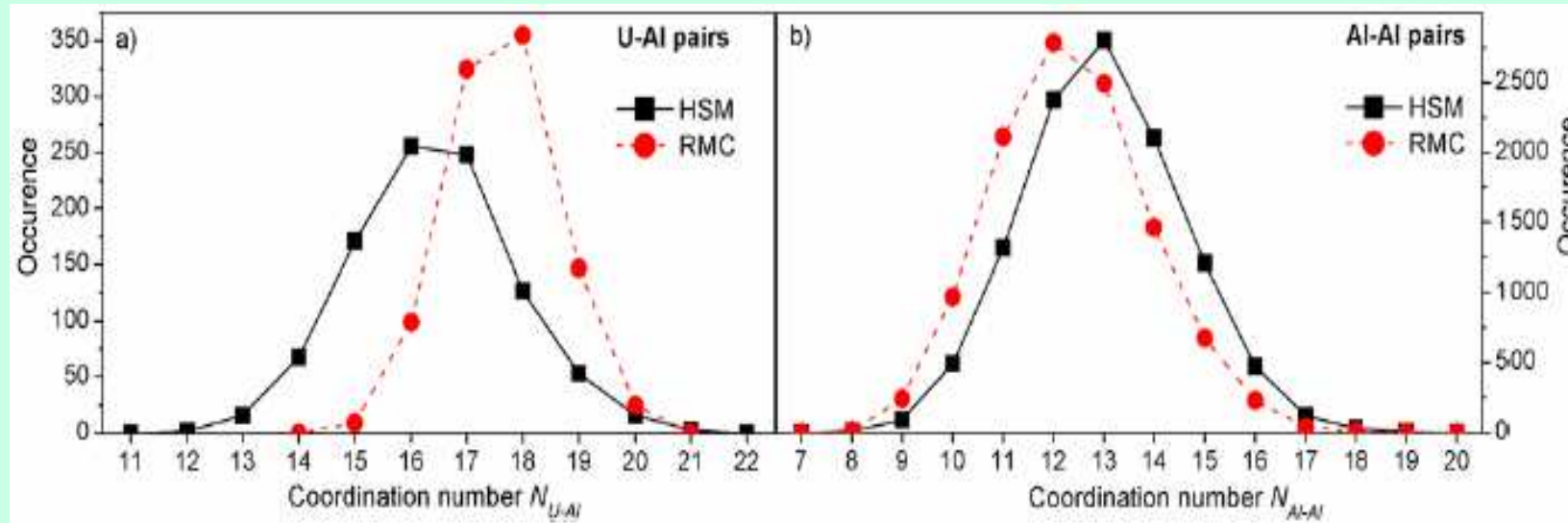
Prírodovedecká fakulta

Múdrost' minulosti – poznatky prítomnosti – vzdelanie budúcnosti.



# RMC modeling

Distributions of coordination numbers can be evaluated !!!



28 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
www.science.upjs.sk



UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH

Prírodovedecká fakulta

Múdrosť minulosti – poznatky prítomnosti – vzdelanie budúcnosti.



# Conclusions

- high energy x-ray diffraction: from the structural factor  $S(Q)$ , the pair distribution function  $D(r)$  is calculated → a local atomic arrangement around an average atom is seen and long range correlations are detectable.
- x-ray absorption spectroscopy: an element sensitive method, the nearest neighbouring of a specific type of atoms is observable.
- Combination of XRD and XAFS: compact information about amorphous structure can be obtained.
- Reverse Monte Carlo simulation is a method which can be used for modelling of a 3D disordered structure in a real space.



**30** 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
[www.science.upjs.sk](http://www.science.upjs.sk)



UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH  
Prírodovedecká fakulta

Múdrosť minulosti – poznatky prítomnosti – vzdelanie budúcnosti.



**31** 18.2.2011

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
[www.science.upjs.sk](http://www.science.upjs.sk)



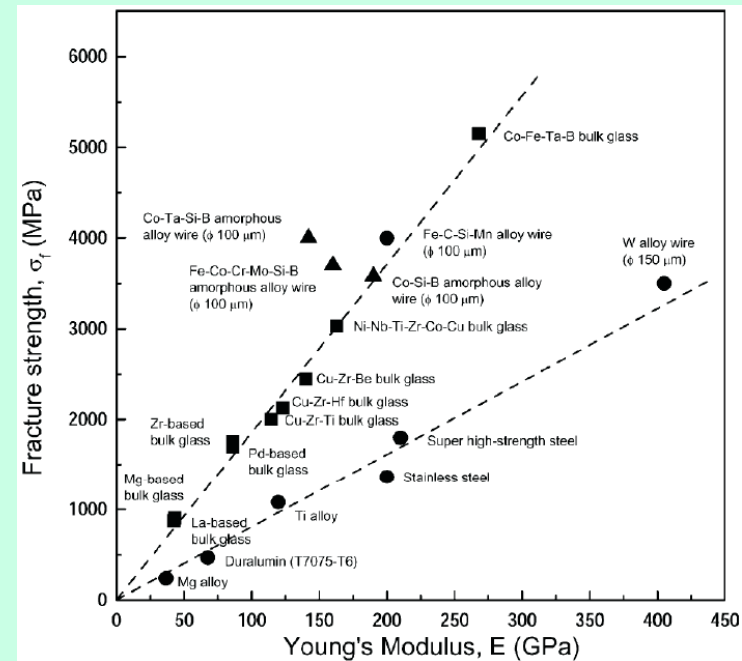
UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH  
Prírodovedecká fakulta

Múdrosť minulosti – poznatky prítomnosti – vzdelanie budúcnosti.



# Prečo kovové sklá?

- Výborné mechanické vlastnosti  
vysoké hodnoty medzi pevnosti, lomovej húževnatosti, tvrdosti, výborné elastické vlastnosti...
- Výborné magnetické vlastnosti  
magneticky mäkké materiály
- Výborné antikorózne vlastnosti
- Zaujímavé termodynamické vlastnosti  
existencia teploty sklenia  $T_g$ , výrazný pokles viskozity, ľahká tvarovateľnosť materiálu



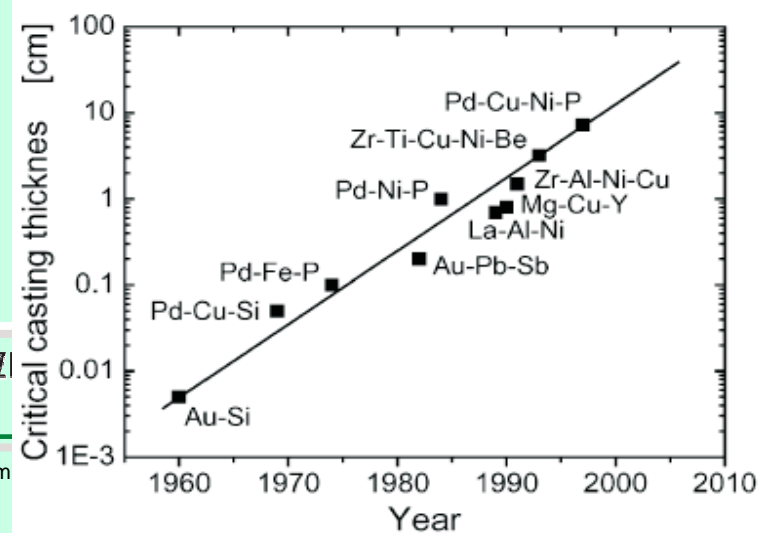
## Nevýhody

- obmedzená schopnosť sklenia
- neexistencia oblasti plastickej deformácie



UNIVERZ

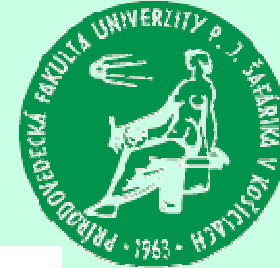
Múdrost' m





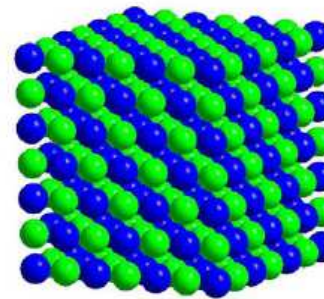
# Predmet môjho štúdia

Charakterizácia neusporiadanej štruktúry kovových skiel s využitím vysoko intenzívnych röntgenových zdrojov

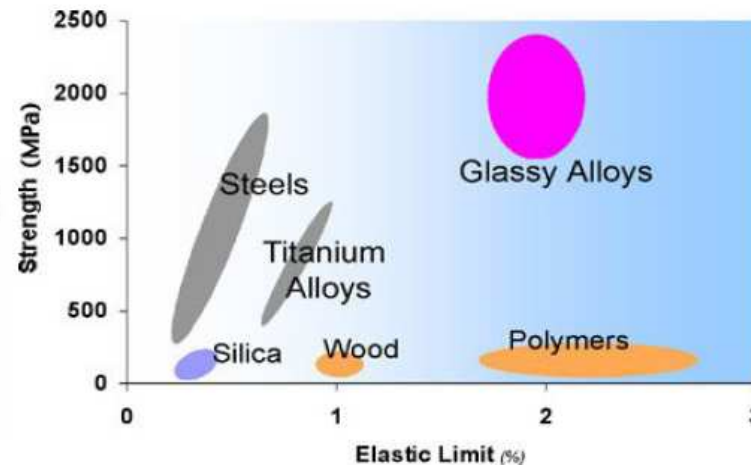
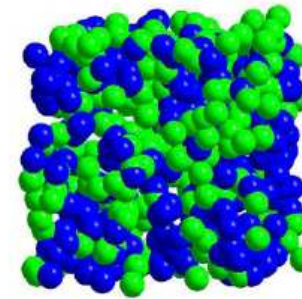


**Metallic glasses** are a new class of engineering materials having an amorphous structure on atomic level and unlike metals, they can be easily deformed at high temperature.

crystalline



amorphous



RNDr. Štefan Michalik  
26.10.2010 v Košiciach

PF UPJŠ v Košiciach  
Moyzesova 16, 041 54 Košice  
www.science.upjs.sk



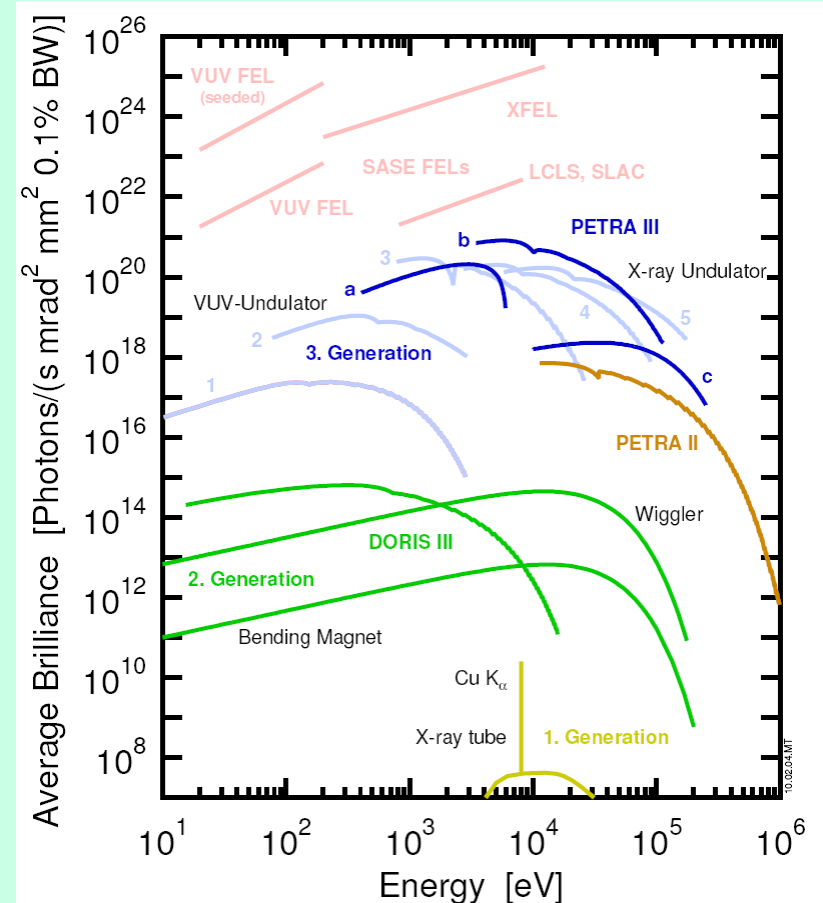
UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH  
Prírodovedecká fakulta

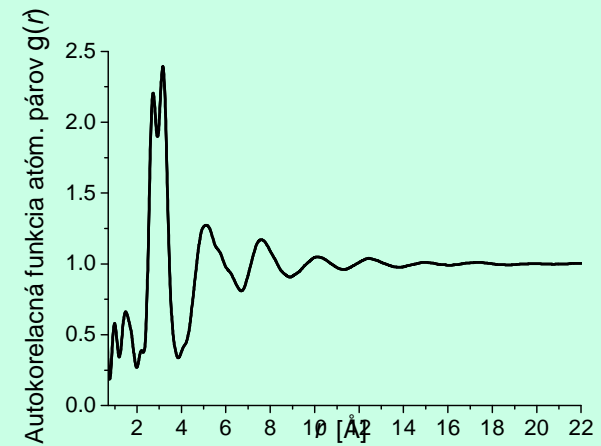


Múdrost' minulosti – poznatky prítomnosti – vzdelanie budúcnosti.

# Zhrnutie: vlastnosti SŽ

- vysoká intenzita
- nízka emitancia, SŽ je takmer úplne kolimované
- vysoký stupeň lineárnej alebo eliptickej polarizácie
- široké a spojité energetické spektrum
- pulzný charakter žiarenia na úrovni nanosekúnd





35 18.2.2011

PF UPJŠ v Košiciach  
 Moyzesova 16, 041 54 Košice  
[www.science.upjs.sk](http://www.science.upjs.sk)



UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH  
 Prírodovedecká fakulta



Múdrosť minulosti – poznatky prítomnosti – vzdelanie budúcnosti.