

Microstructural parameters from *Multiple Whole Profile (MWP)* or *Convolutional Multiple Whole Profile (CMWP)* computer programs

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Line Profile Analysis Workshop

Tutorial outline:

- 1) Brief theoretical background,
- 2) Microstructural parameters,
- 3) Determining the dislocations types,
 - 1) cubic crystal system,
 - 2) hexagonal crystal system,
- 4) MWP (**M**ultiple **W**hole **P**rofile **F**itting),
- 5) CMWP (**C**onvolutional **M**ultiple **W**hole **P**rofile **F**itting),
- 6) ANIZC – program,
- 7) Examples,
- 8) Summary.

MWP and CMWP-fit

MWP and CMWP-fit are computer programs developed by *Prof. Ungar Tamas* and *Dr. Ribarik Gabor* (Diffraction Laboratory, Department of General Physics at Eotvos Science University in Budapest, Hungary) for the determining the microstructural parameters from X-ray diffraction patterns of materials with cubic or hexagonal crystal lattice.

The programs are available for on-line usage at:

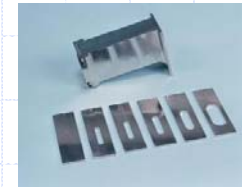
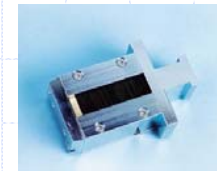
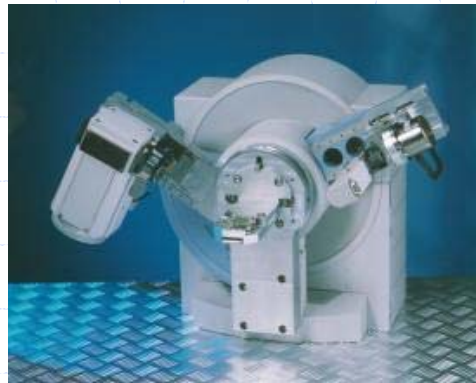
<http://www.renyi.hu/cmwp/>

<http://www.renyi.hu/mwp/>

Sources of X-ray Line Broadening:

Instrumental sources: broadening caused by diffractometer imperfections

(Non ideal optics, Wavelength Dispersion, Sample Transparency, Axial Divergence, Detector resolution)



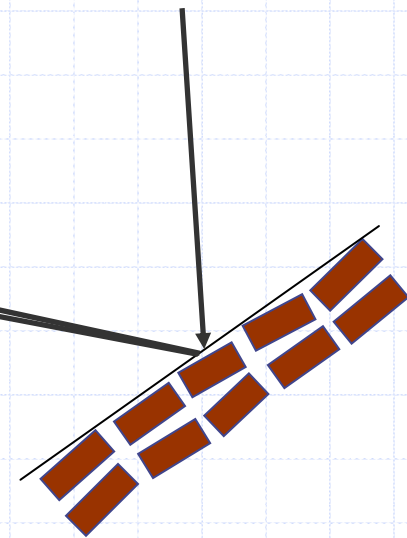
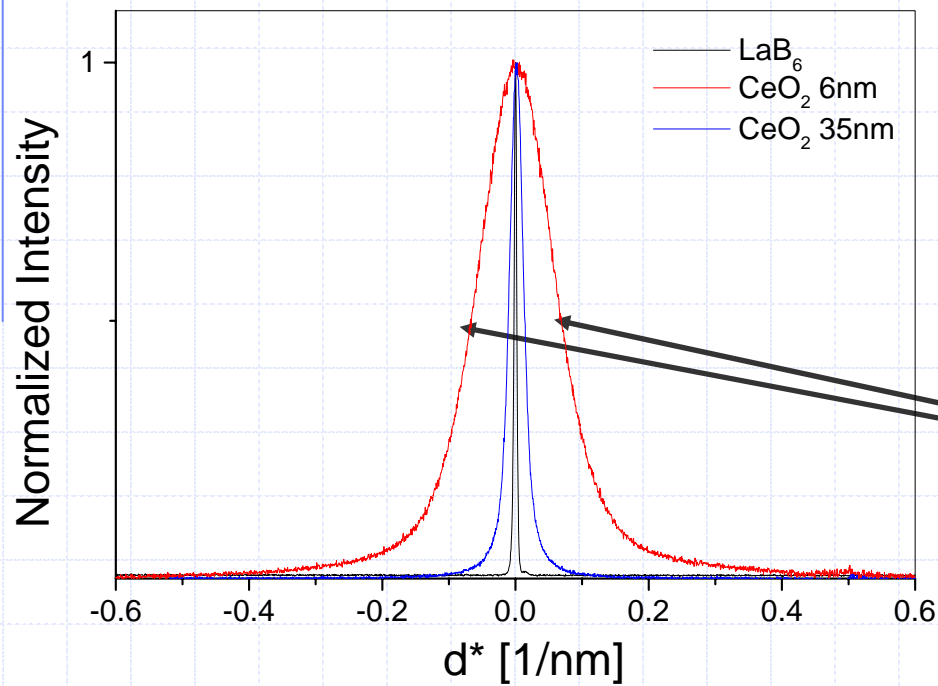
Standards for instrumental broadening: SRM660a (LaB₆), SRM640c (Si) - NIST

Standard specimen preparation: Berkum, J. G. M. van, Sprong, G. J. M., Keijser, Th. H. de, Delhez, R. and

Sonneveld, E. J. (1995), Powder Diffr. 10, 129-139

Physical sources X-ray line profile broadening :

- broadening effect due to crystallite smallness (coherent domain).



Coherent domain X-ray line broadening may include effects of stacking- and twin faults and sub-grain structures (for instance small-angle grain boundaries).

Physical sources X-ray line profile broadening :

- broadening effect due to micro-strain:
 - dislocations,
 - stacking faults,
 - precipitates of second phase particles,
 - concentration gradients in solid solutions,
 - severely distorted grain boundaries in nano-crystalline materials,
 - different types of internal stresses or strains which may be heterogeneous.

X-ray Line Broadening

$$I_m = I_{\text{instrumental}} * I_{\text{size}} * I_{\text{distorsion}} * I_{\text{other}}$$

MWP and CMWP-fit - theoretical background

Assumptions:

- 1) X-ray diffraction line is broadened due to:
 - small coherent domains (usually smaller than $1\ \mu\text{m}$),
 - lattice distortion.
- 2) The crystallites are spherical or ellipsoidal,
- 3) The crystallite size distribution is lognormal.
- 4) The lattice distortion is assumed to be caused by dislocations

MWP and CMWP-fit - theoretical background

- *Physical* profile functions - $I_m = I_{\text{size}} * I_{\text{distorsion}}$

Size effect:

Assumption → log-normal size distribution and spherical crystallites:

$$I_{\text{size}}(s) = \int_0^{\infty} \mu \frac{\sin^2(\mu \pi s)}{(\pi s)^2} \operatorname{erfc} \left[\frac{\log \left(\frac{\mu}{m} \right)}{\sqrt{2}\sigma} \right] d\mu,$$

where m is the median, σ is the variance of the log-normal size distribution and erfc is the complementary error function.

MWP-fit - theoretical background

- *Physical* profile functions - $I_m = I_{\text{size}} * I_{\text{distorsion}}$

$$A(L) = A^{\text{size}}(L) A^{\text{distorsion}}(L)$$

Strain effect - dislocations:

Based on the Wilkens model (1970) the Fourier transform of the strain profiles are written as:

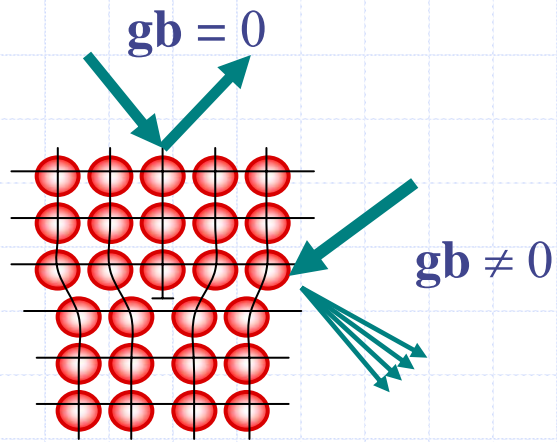
$$A^D(L) = \exp\{-2\pi^2 g^2 L^2 [(b/2\pi)^2 \pi \rho \bar{C} f(L/R_e^*)]\}$$

where g is the absolute value of the diffraction vector; L is the Fourier length, b is the absolute value of the Burgers vector, ρ is the dislocation density; \bar{C} is the average contrast factor of dislocation; R_e^* is the effective outer cut-off radius and f is the Wilkens function.

Strain effect - dislocations

Strain anisotropy

Similar to TEM



MWP - fit:

The Fourier transforms of the measured profiles are fitted all at once with:

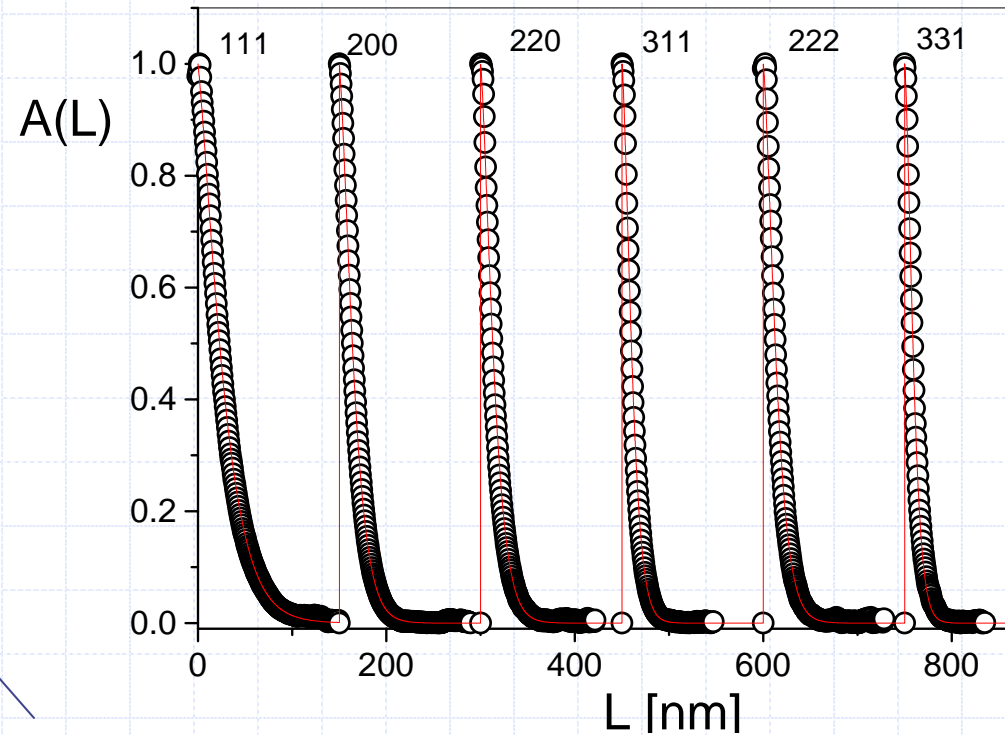
$$A(L) = \left[A^s(L) / A^s(0) \right] \exp \left\{ -2\pi^2 g^2 L^2 \left[(b / 2\pi)^2 \pi \rho \bar{C} f(L / R_e^*) \right] \right\}$$

MWP - fit:

$$A_L = A_L^S A_L^D(hkl)$$

log-normal size
distribution: $\Rightarrow m$ and σ

strain in terms of dislocations
 $\Rightarrow \rho$ and M
 \Rightarrow Strain anisotropy: $C_{av}(\mathbf{q}, c_{ij})$



Nonlinear least squares method:

$$(A^{(\text{meas})} - A^{(\text{calc})})^2 = \min.$$

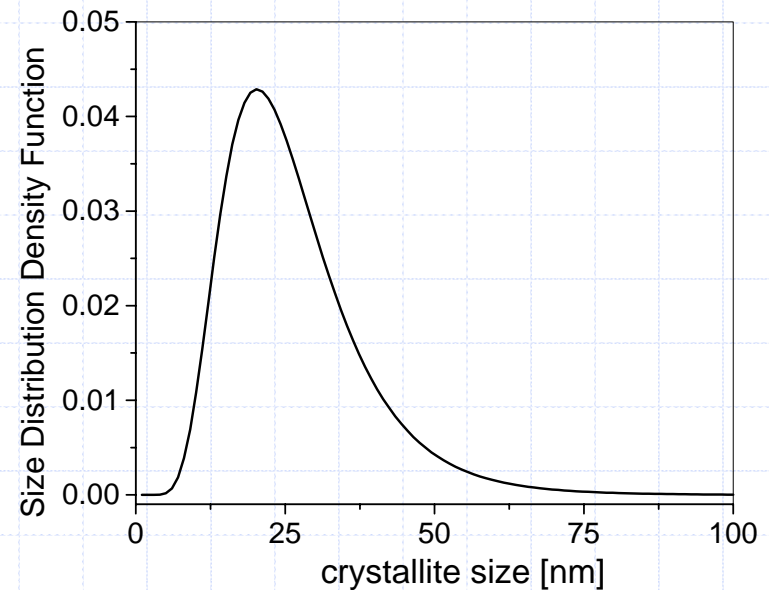
Microstructural parameters obtained from MWP and CMWP procedures – m and σ

Crystallite size distribution:

The procedure assumes lognormal size distribution with spherical or ellipsoidal crystallite shape.

spherical crystallites:

$$f(x) = \frac{1}{(2\pi)^{1/2}} \frac{1}{\sigma x} \exp\left\{-\frac{[\log(x/m)]^2}{2\sigma^2}\right\}$$



Strain anisotropy parameter, q :

Average contrast factors of dislocations for **cubic** crystal systems:

$$\bar{C} = \overline{C_{h00}} (1 - q \cdot H^2)$$

where $H^2 = (h^2k^2 + h^2l^2 + k^2l^2) / (h^2 + k^2 + l^2)^2$

- q depends on the
- studied material **elastic properties**,
 - dislocation geometry/character**.

Microstructural parameters obtained from MWP and CMWP procedures:

Strain anisotropy parameter, q : $\bar{C} = \overline{C_{h00}} (1 - q \cdot H^2)$

1) If the dislocation structure is known from other techniques, such as TEM, than the C_{h00} and q can be numerically calculated for the given dislocation structure and inputted as a fix parameters in the MWP or CMWP procedure.

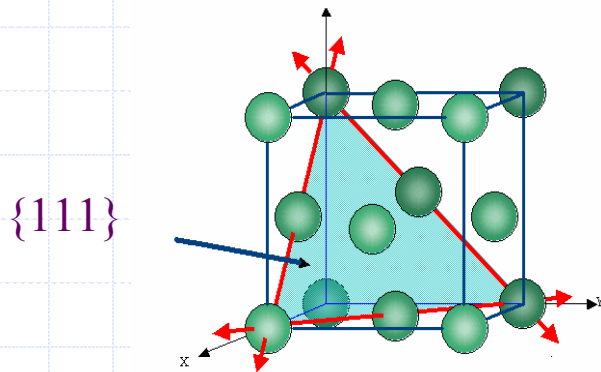
2) If the dislocation structure is unknown, than in the MWP or CMWP procedures C_{h00} is fixed while the q is refined. From the value of q the dislocations type/population can determined and the real C_{h00} can be obtained.

Microstructural parameters obtained from MWP and CMWP procedures:

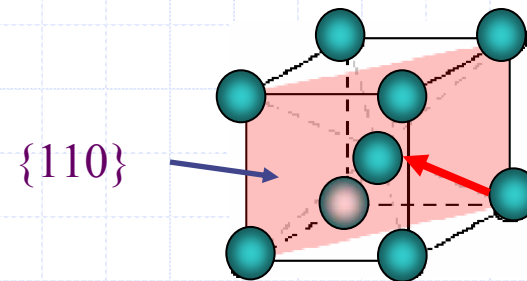
Strain anisotropy parameter, q :

determining the dislocations character

FCC: $a/2 \langle 110 \rangle \{111\}$



BCC: $a/2 \langle 111 \rangle \{110\}$
 $a/2 \langle 111 \rangle \{112\}$



Theoretical individual and average contrast factor of dislocations can be found in:

Ungár, T., Dragomir, I., Révész, Á., and Borbély, A.: “The Contrast Factors of Dislocations in Cubic Crystals: the Dislocation Model of Strain Anisotropy in Practice”, *J. Appl. Cryst.*, 32, 992-1002, (1999).

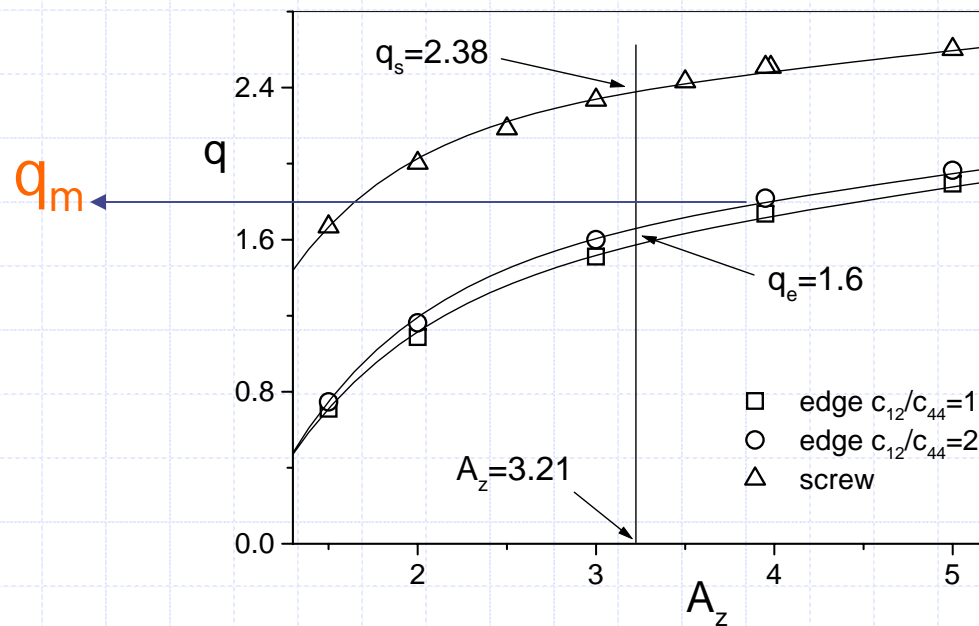
Dragomir I. C. and Ungár T.: “The dislocations contrast factors of cubic crystals in the Zener constant range between zero and unity” in *Powder Diffraction Journal*, 17, 104-111, (2002).

Microstructural parameters obtained from MWP and CMWP procedures:

Cubic crystal systems – theoretical average dislocation contrast factor:

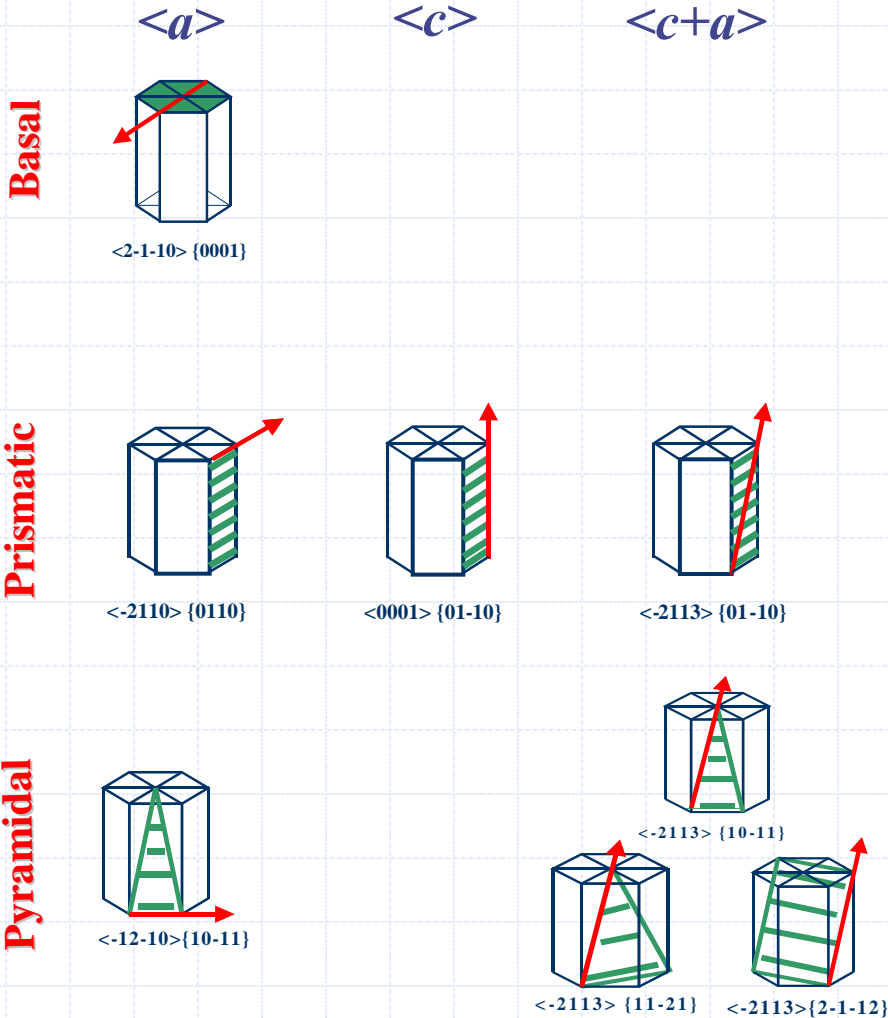
FCC system - dislocation slip systems: $1/2\langle 110 \rangle \{111\}$ type

$$q_m = f q_e + (1-f) q_s$$



Average dislocation contrast factor for hexagonal crystal systems:

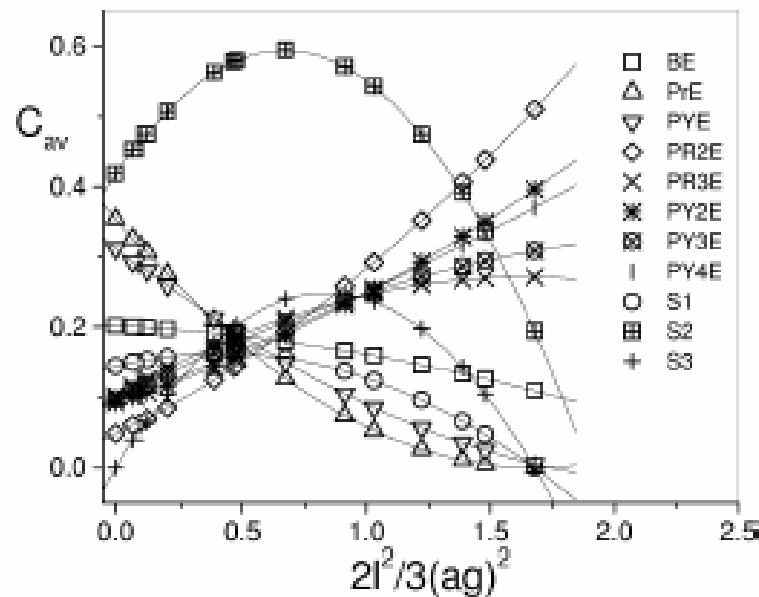
Dislocation slip systems



Microstructural parameters obtained from MWP and CMWP procedures:

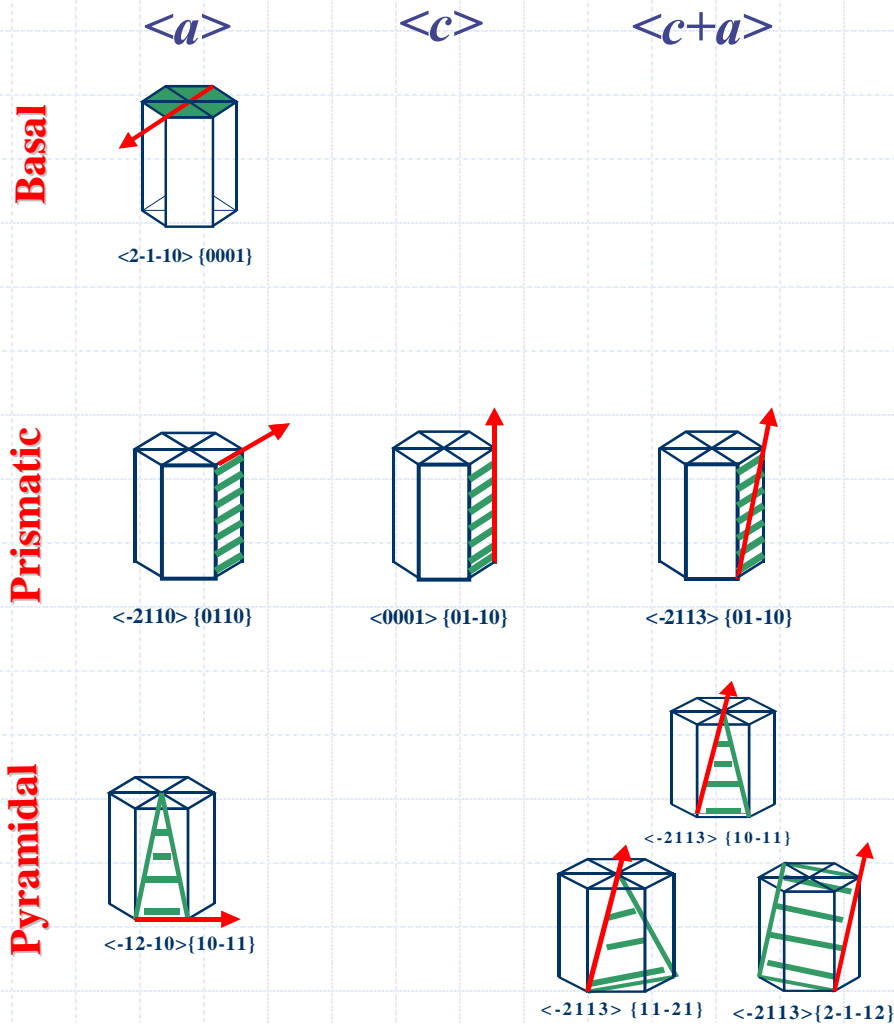
Average contrast factor for hexagonal crystal systems, q_1 and q_2 :

$$\bar{C}_{hk.l} = \bar{C}_{hk.0} [1 + q_1 x + q_2 x^2],$$



Dragomir I. C. and Ungár T.: “The contrast factors of dislocations in the hexagonal crystal system” in J. Appl. Cryst., 35, 556-564, (2002).

To many unknowns – assumptions are needed



Microstructural parameters obtained from MWP and CMWP procedures:

Hexagonal crystal systems, q_1 and q_2 :

Measured and Theoretical average contrast factor of dislocations:

$$\begin{aligned} C_m &= f_1 C_1 + f_2 C_2 + f_3 C_3 \\ f_1 + f_2 + f_3 &= 1 \end{aligned}$$

→

$$q_1^{(m)} = \frac{1}{P} \sum_{i=1}^3 h_i \overline{C}_{hk.0}^{(i)} b_i^2 q_1^{(i)},$$

$$q_2^{(m)} = \frac{1}{P} \sum_{i=1}^3 h_i \overline{C}_{hk.0}^{(i)} b_i^2 q_2^{(i)},$$

$$\sum_{i=1}^3 h_i = 1,$$

$$\text{where } P = \sum_{i=1}^3 h_i \overline{C}_{hk.0}^{(i)} b_i^2 = \overline{b^2 C}_{hk.0}^{(m)}.$$

Microstructural parameters obtained from MWP and CMWP procedures – dislocation density

Evaluation of real dislocation density, ρ :

Cubic: $\dots \rho \bar{C} = \dots \overline{\rho C_{h00}} (1 - q \cdot H^2)$

$$\rho^* \cdot \bar{C}_{h00}^{(input)} = \rho \cdot \bar{C}_{h00}^{(real)}$$

Hexagonal: $\dots \rho b^2 \bar{C} = \dots \overline{\rho b^2 C_{hk0}} (1 + q_1 x + q_2 x^2)$

$$b^2 \overline{C_{hk.0}}^{(input)} \cdot \rho^* = \overline{b^2 C_{hk.0}}^{(real)} \cdot \rho$$

Microstructural parameters obtained from MWP and CMWP procedures – arrangement parameter

Dislocation arrangement parameter, M (Wilkins, 1970):

M is defined by Wilkins as the dislocation arrangement parameter.

$$M = R_e \sqrt{\rho}$$

$M \gg 1$ weak screening of dislocations fields

$M \sim 1$ quasi-homogeneous dislocation arrangement

$M \ll 1$ strong screening of dislocations fields, dipole configurations

MWP-fit:

Before using MWP the following profile corrections are necessary:

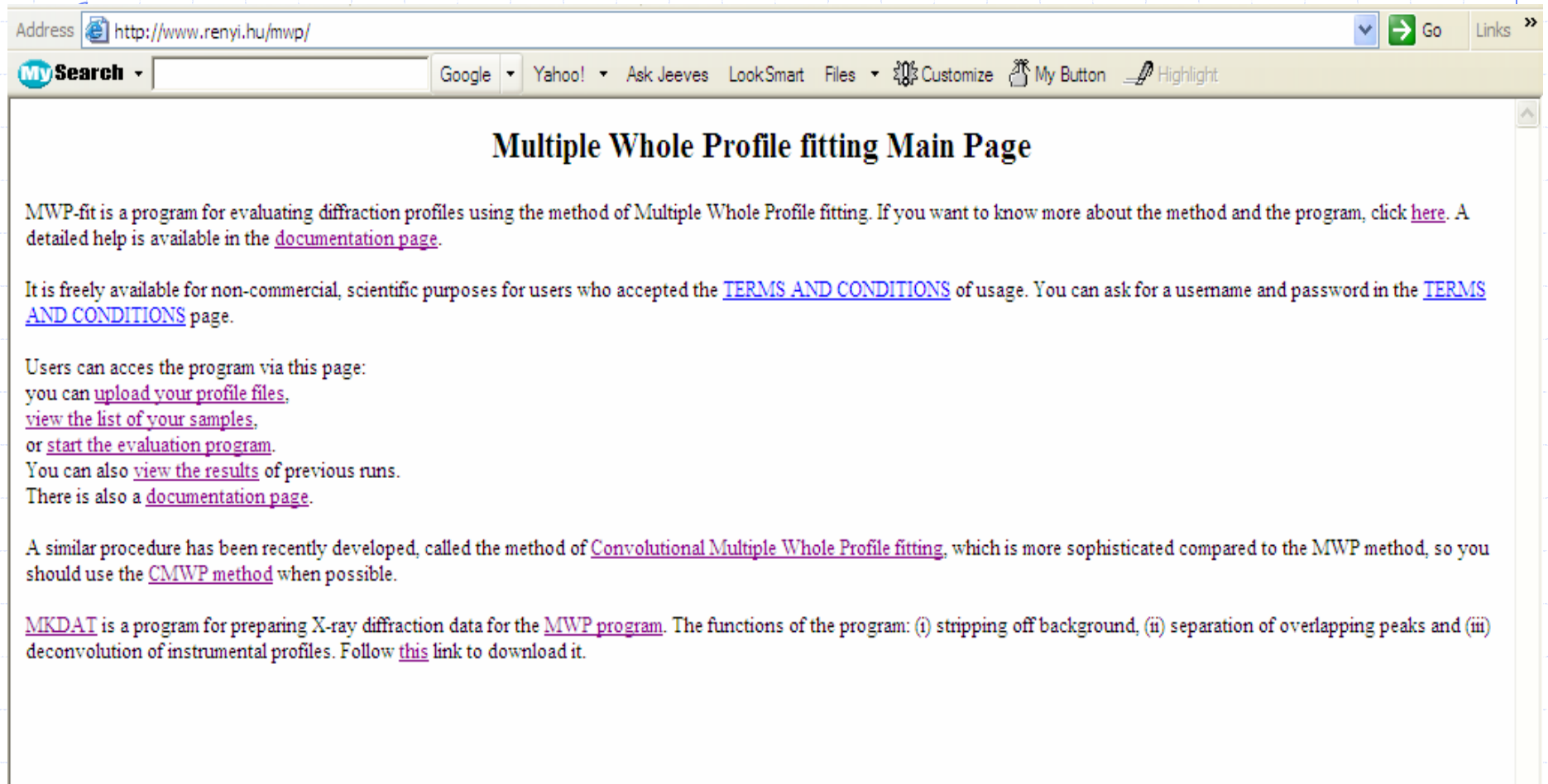
- i) background
- ii) overlapping peaks
- iii) $K\alpha_2$
- iv) instrumental effect

Free software: MKDAT at <http://www.renyi.hu/mkdat>

Other free software that can be used for corrections can be found at:
<http://www.ccp14.ac.uk/>

Also commercial software as Jade, Topas, High Score Plus, etc.

MWP – fit front-end:



The screenshot shows a web browser window with the address bar containing "http://www.renyi.hu/mwp/". The browser's search bar is set to "My Search" and includes links to Google, Yahoo!, Ask Jeeves, and LookSmart. The main content area of the page is titled "Multiple Whole Profile fitting Main Page".

MWP-fit is a program for evaluating diffraction profiles using the method of Multiple Whole Profile fitting. If you want to know more about the method and the program, click [here](#). A detailed help is available in the [documentation page](#).

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Users can access the program via this page:
you can [upload your profile files](#),
[view the list of your samples](#),
or [start the evaluation program](#).
You can also [view the results](#) of previous runs.
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A similar procedure has been recently developed, called the method of [Convolutional Multiple Whole Profile fitting](#), which is more sophisticated compared to the MWP method, so you should use the [CMWP method](#) when possible.

[MKDAT](#) is a program for preparing X-ray diffraction data for the [MWP program](#). The functions of the program: (i) stripping off background, (ii) separation of overlapping peaks and (iii) deconvolution of instrumental profiles. Follow [this](#) link to download it.

MWP - fit - Input files

Format: 2-column ASCII type of files for every *hkl* diffraction profile

1) The first column contains :

$$d^* = 1/d = 2\sin(\theta - \theta_0) / \lambda$$

2) The second column contains the normalized intensity.

Example:

-0.0023	0.981756
-0.0018	0.989999
-0.0013	0.995834
-0.0009	0.999185
-0.0004	0.998253
0	1
0.0004	0.993943
0.0009	0.9871
0.0013	0.977779
0.0018	0.966061
0.0023	0.952054

MWP procedure:

Input files - examples

The screenshot shows a web browser window with the address bar containing `http://www.renyi.hu/mwp/program/mwp-upload.html`. The page title is "MWP-fit Upload Page". Below the title, there is a paragraph of instructions: "Here you can transfer the intensity profiles or their Fourier transforms from your computer to your main directory with this simple tool. Specify the name of your sample (the name of the directory in which the profiles will be uploaded), specify the hkl-indices, click on **Browse...** to select the files and then click **Upload Files**." Below this, there is a form with a text input field for "Name of the sample:" containing the text "CeO2-1". There is also a checkbox labeled "The files are Fourier transforms instead of intensity profiles:" which is currently unchecked. Below the checkbox, there is a list of hkl indices and their corresponding filenames, each with a "Browse..." button next to it. The list includes hkl values 111, 200, 220, 222, 311, 331, 400, 420, 422, and 440. At the bottom of the form, there are two buttons: "Upload Files" and "Clear". Below the form, there is a link: "Click [here](#) to start the evaluation procedure."

Address `http://www.renyi.hu/mwp/program/mwp-upload.html` Go Links >>

MWP-fit Upload Page

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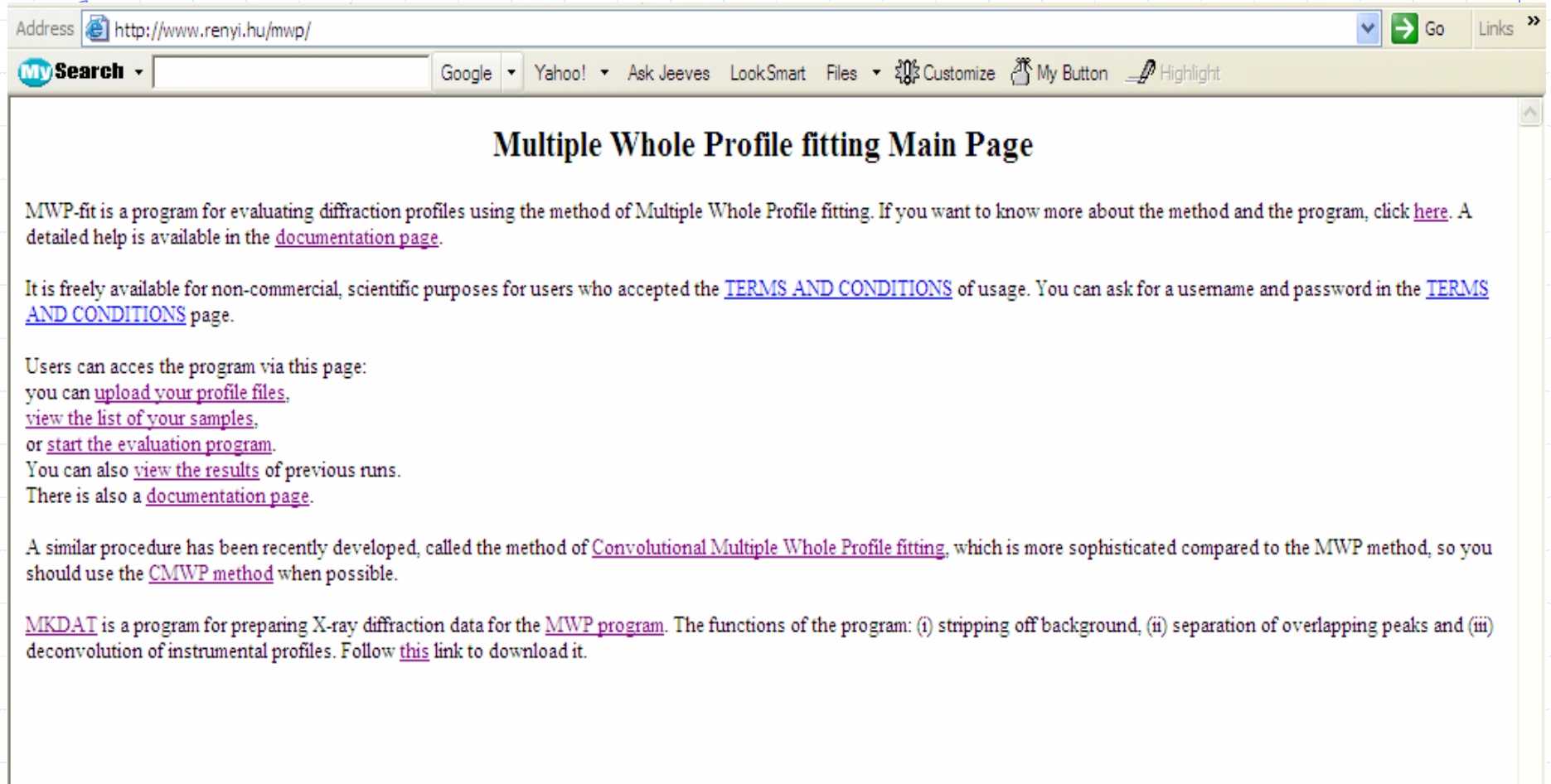
Name of the sample:

The files are Fourier transforms instead of intensity profiles:

hkl: <input type="text" value="111"/>	filename: <input type="text" value="ver\2005\MWP\CeO2\S1\best\111.dat"/>	<input type="button" value="Browse..."/>
hkl: <input type="text" value="200"/>	filename: <input type="text" value="ver\2005\MWP\CeO2\S1\best\200.dat"/>	<input type="button" value="Browse..."/>
hkl: <input type="text" value="220"/>	filename: <input type="text" value="ver\2005\MWP\CeO2\S1\best\220.dat"/>	<input type="button" value="Browse..."/>
hkl: <input type="text" value="222"/>	filename: <input type="text" value="ver\2005\MWP\CeO2\S1\best\222.dat"/>	<input type="button" value="Browse..."/>
hkl: <input type="text" value="311"/>	filename: <input type="text" value="ver\2005\MWP\CeO2\S1\best\311.dat"/>	<input type="button" value="Browse..."/>
hkl: <input type="text" value="331"/>	filename: <input type="text" value="ver\2005\MWP\CeO2\S1\best\331.dat"/>	<input type="button" value="Browse..."/>
hkl: <input type="text" value="400"/>	filename: <input type="text" value="ver\2005\MWP\CeO2\S1\best\400.dat"/>	<input type="button" value="Browse..."/>
hkl: <input type="text" value="420"/>	filename: <input type="text" value="ver\2005\MWP\CeO2\S1\best\420.dat"/>	<input type="button" value="Browse..."/>
hkl: <input type="text" value="422"/>	filename: <input type="text" value="ver\2005\MWP\CeO2\S1\best\422.dat"/>	<input type="button" value="Browse..."/>
hkl: <input type="text" value="440"/>	filename: <input type="text" value="ver\2005\MWP\CeO2\S1\best\440.dat"/>	<input type="button" value="Browse..."/>

Click [here](#) to start the evaluation procedure.

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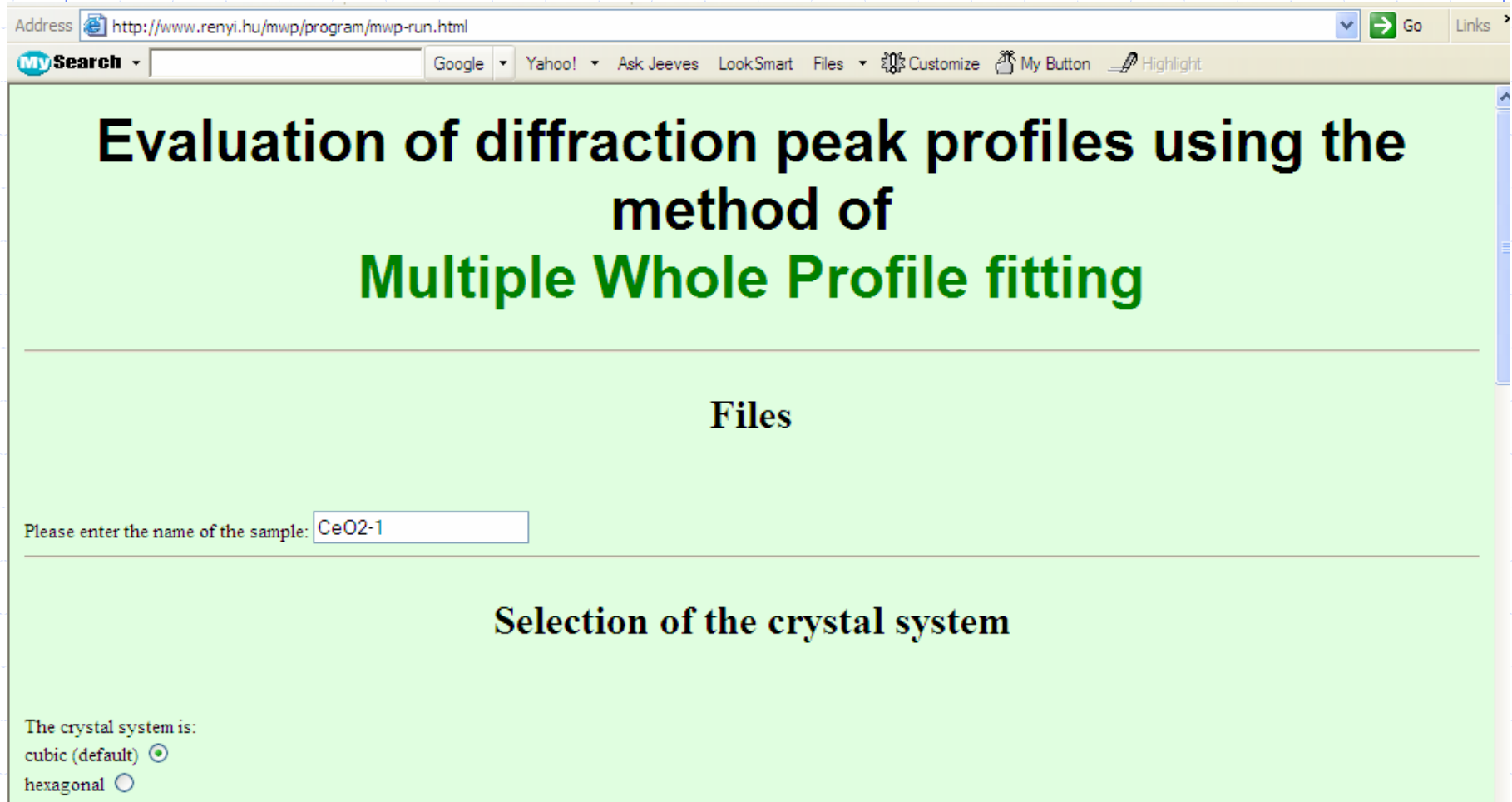
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MWP procedure:

- crystal system selection



Address  http://www.renyi.hu/mwp/program/mwp-run.html  Go Links >

MY Search Google Yahoo! Ask Jeeves LookSmart Files  Customize  My Button  Highlight

Evaluation of diffraction peak profiles using the method of Multiple Whole Profile fitting

Files


Please enter the name of the sample:




Selection of the crystal system

The crystal system is:
cubic (default)
hexagonal

MWP procedure:

- *input parameters*

Address  <http://www.renyi.hu/mwp/program/mwp-run.html>

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Input parameters

Please enter the value of the lattice constant "a" (in nm):

Please enter the value of the lattice constant "c" (in nm):

Please enter the value of the absolute value of the Burgers vector (in nm):

Please enter the average contrast factor of the h00 (or hk0) reflections:

Please note that setting of the lattice parameter "c" has effect only if the crystal system is hexagonal.

Selection of the size function



The program will use the spheric size function (default)




The program will use the ellipsoidal size function

The program will disable the size effect

MWP procedure:

-settings

Address  http://www.renyi.hu/mwp/program/mwp-run.html  Go Links >>

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Sampling of the Fourier transform of the measured data

Please specify the number of samples:

Please specify the upper limit of sampling (in FWHM units):

Please specify the maximal frequency used for plotting and/or sampling the input data:

The program will recompute the Fourier transforms using the new settings:

Initial values of the parameters

Please enter the initial value of the parameter "a" (or "a1"): fix:

Please enter the initial value of the parameter "a2": fix:

Please enter the initial value of the parameter "b": fix:

Please enter the initial value of the parameter "c": fix:

Please enter the initial value of the parameter "d": fix:

Please enter the initial value of the parameter "e": fix:

Please enter the initial value of the parameter "epsilon": fix:

fix d*e:

Please note that setting of the parameter "a2" has effect only if the crystal system is hexagonal and setting of the parameter "epsilon" has effect only if the size function is ellipsoidal.

MWP procedure:

Selection of the method of fitting

The program will fit the intensity profiles instead of the Fourier Transforms

Fit control


Please specify the limit for stopping:

Please specify the maximal number of iterations:

After filling in the relevant fields in this form, please press/click this button: to begin the evaluation procedure. Click the button to reset the values.

Done

Internet

Address  http://www.renyi.hu/cgi-bin/post-mwp?SAMPLENAME=CeO2-1&HEXAGONAL_CRYSTAL=n&a=0.3604&c=1.0&bb=0.254841&C0=0.3040&N=256&FOURIER_FWH


Multiple Whole Profile fitting

Connecting the server for evaluation

The evaluation is started.

Please wait until this page loads to get the results.

Note that the results will be stored in <http://www.renyi.hu/mwp/results/dragomir/CeO2-1-2005-08-02-05-46-33>.

Address  http://www.renyi.hu/cgi-bin/post-mwp?SAMPLENAME=CeO2-1&HEXAGONAL_CRYSTAL=n&a=0.3604&c=1.0&bb=0.254841&C0=0.3040&N

Multiple Whole Profile fitting

Connecting the server for evaluation
The evaluation is started.
Please wait until this page loads to get the results.

Note that the results will be stored in <http://www.renyi.hu/mwp/results/dragomir/CeO2-1-2005-08-02-05-46-33>.

The fitting is done, evaluate's output follows:

```
This is MWP-fit, a program for Multiple Whole Profile Fitting using
theoretical line profile functions.
Copyright (C) Gábor Ribárik and Tamás Ungár, 1998-2000. All rights reserved.
For permission to use, copy, modify this program or any of its components,
ask the authors. Redistributing this software is not allowed.
```


```
Date: 2005-08-02 05:46:34
```


```
Data directory: dragomir/CeO2-1
```

```
The value of the lattice constant (in nm): 0.3604
The absolute value of the Burgers vector (in nm): 0.254841
The average contrast factor of the h00 reflections: 0.3040
The definition of the Size Function:
sf_spheric(k,b,c)=Int(0.5*x*erfc((log(x)-b)/c)*(sin(Pi*k*x)/(Pi*k))**2,x=0..Inf)
```

```
Common characteristics of the Fourier Spectrums:
The number of samples: 256
The upper limit of sampling (in FWHM units): 5
The maximal frequency used for sampling and/or plotting: 220
```

```
*** FIT ***
```

 Done

Address  http://www.renyi.hu/cgi-bin/post-mwp?SAMPLENAME=CeO2-1&HEXAGONAL_CRYSTAL=n&a=0.3604&c=1.0&bb=0.2548

*** FIT ***

Calculating a,b,c,d,e to fit the Fourier Spectrums with:
(fct(x)/fct(0))*exp(-(K^2*C*x^2/d^2)*wf(e*x)), where fct(x) is the Fourier
Transform of sf_spheric(x,b,c), $K^2=(h^2+k^2+l^2)/a^2$, $C=Ch00*(1-a*H^2)$,
 $H^2=(h^2*k^2+h^2*l^2+k^2*l^2)/(h^2+k^2+l^2)^2$ and wf(x)=f^(x) as defined
by M. Wilkens in:
Proc. Conf. Fund. Aspects of Disl. Theory, National Bureau of Standards, 1969.

The initial values of the parameters:

C0=0.3040
a = 2.0
b = 3.0
c = 1.0
d = 80.0
e = 0.05
epsilon = 1.0 # FIXED

The solutions:

a=2.32832
b=3.27845
c=0.55576
d=11.089
e=44.5776

m=exp(b)=26.5346
sigma=c/sqrt(2)=0.392982
D=41.255847401345nm
d=34.168nm
L0=26.0254nm

q=a=2.32832
rho=2/(Pi*(0.254841nm*d)**2)=0.0797181(1/nm)^2
Re^*=exp(-1/4)/(2*e)=0.00873534nm
M^*=(Re^*)*sqrt(rho)=0.00246637

After 732 iterations the fit converged.
final sum of squares of residuals : 5.29228
rel. change during last iteration : -4.48066e-10

 Done

Address http://www.renyi.hu/cgi-bin/post-mwp?SAMPLENAME=CeO2-1&HEXAGONAL_CRYSTAL=n&a=0.3604&c=1.08&bb=0.254841&c0=0.3040&N=256&FOURIER_FV

e=44.5776

m=exp(b)=26.5346
sigma=c/sqrt(2)=0.392982
D=41.255847401345nm
d=34.168nm
L0=26.0254nm

q=a=2.32832
rho=2/(Pi*(0.254841nm*d)**2)=0.0797181(1/nm)^2
Re^*=exp(-1/4)/(2*e)=0.00873534nm
M^*=(Re^*)*sqrt(rho)=0.00246637

After 732 iterations the fit converged.

final sum of squares of residuals : 5.29228

rel. change during last iteration : -4.48066e-10

Final set of parameters Asymptotic Standard Error

	Final set of parameters		Asymptotic Standard Error	
	=====		=====	
a	= 2.32832	+/- 0.1804	(7.748%)	
b	= 3.27845	+/- 0.03636	(1.109%)	
c	= 0.55576	+/- 0.01891	(3.403%)	
d	= 11.089	+/- 248.3	(2239%)	
e	= 44.5776	+/- 1999	(4485%)	

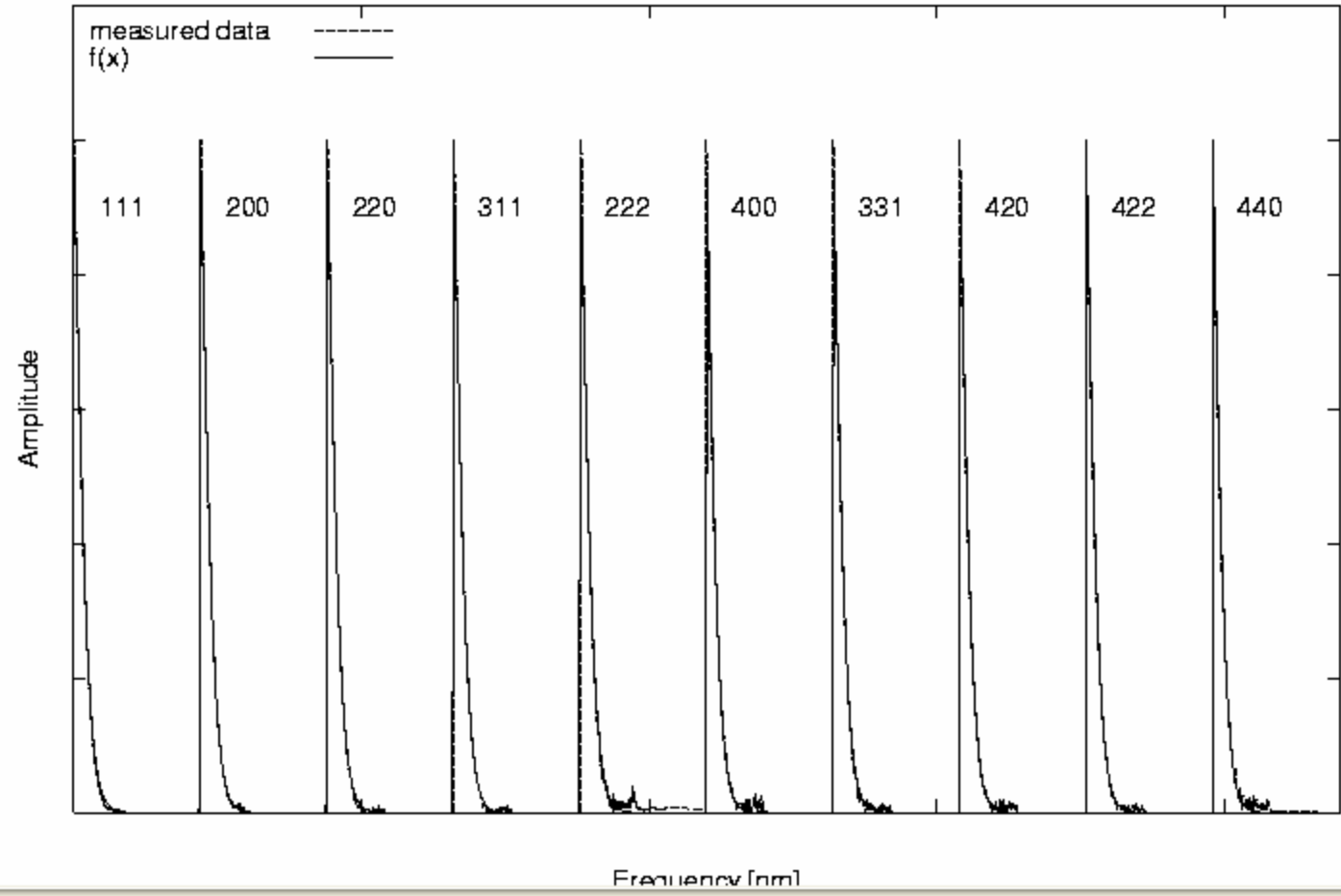
For more information about correlation matrix and confidence intervals,
please read the file dragomir/CeO2-1.fourier.sol.

*** END OF FITTING ***

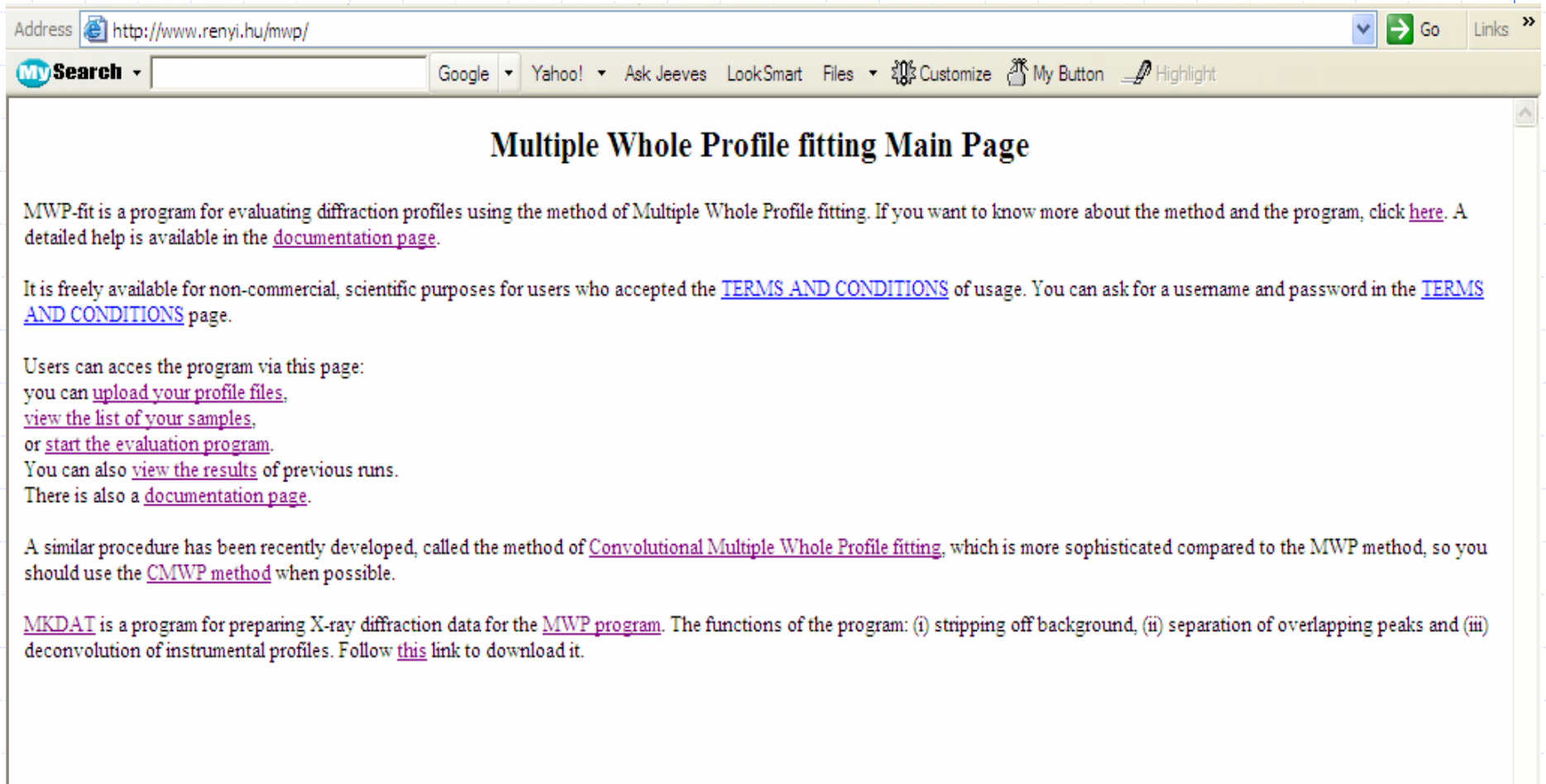
Fourier Transform of dragomir/CeO2-1

Done

Fourier Transform of dragomir/CeO2-1



MWP procedure:



The screenshot shows a web browser window with the address bar containing "http://www.renyi.hu/mwp/". The browser's search bar is set to "mySearch" and includes links to Google, Yahoo!, Ask Jeeves, LookSmart, and Files. There are also icons for "Customize", "My Button", and "Highlight". The main content area of the browser displays the "Multiple Whole Profile fitting Main Page".

Multiple Whole Profile fitting Main Page

MWP-fit is a program for evaluating diffraction profiles using the method of Multiple Whole Profile fitting. If you want to know more about the method and the program, click [here](#). A detailed help is available in the [documentation page](#).

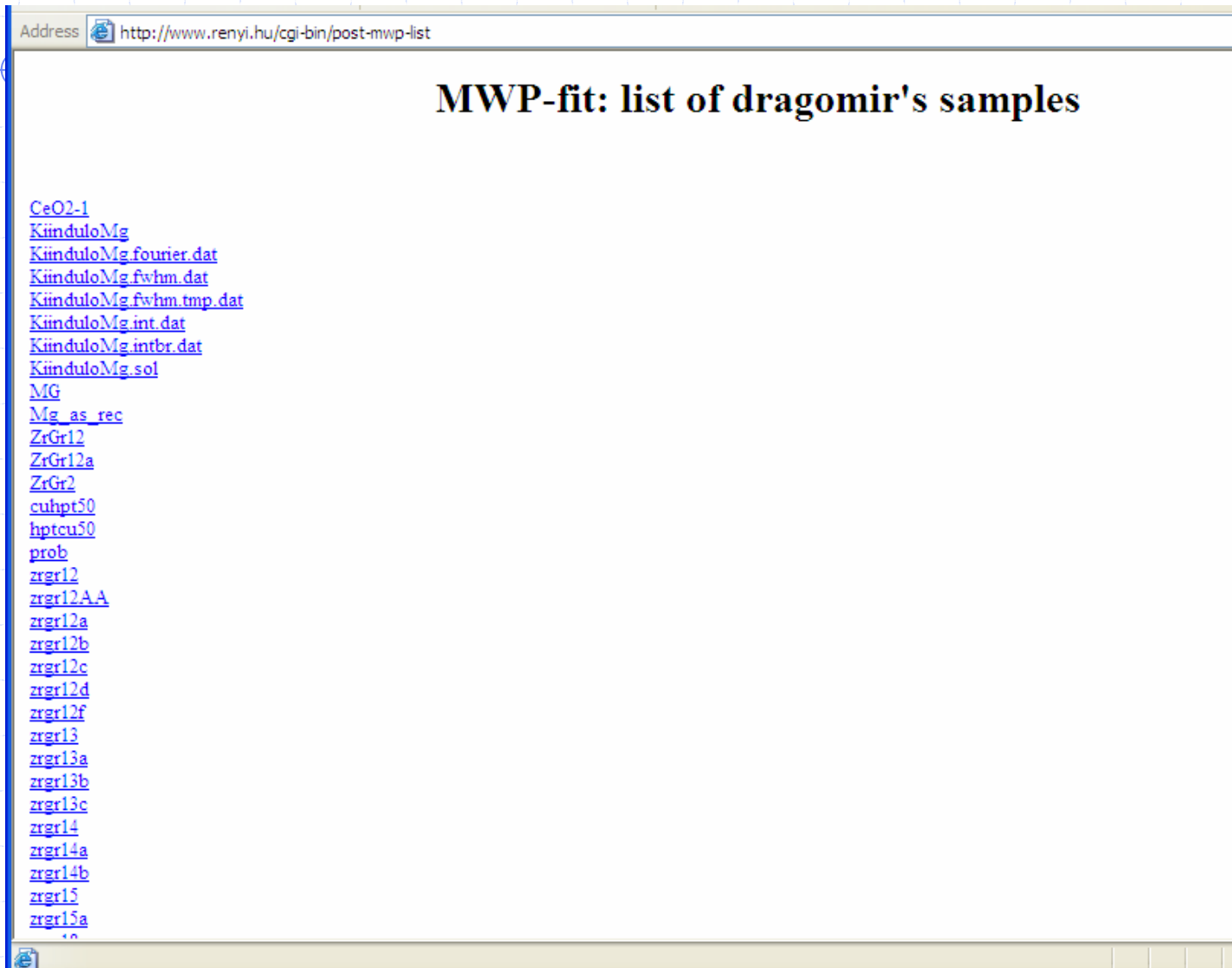
It is freely available for non-commercial, scientific purposes for users who accepted the [TERMS AND CONDITIONS](#) of usage. You can ask for a username and password in the [TERMS AND CONDITIONS](#) page.

Users can access the program via this page:
you can [upload your profile files](#),
[view the list of your samples](#),
or [start the evaluation program](#).
You can also [view the results](#) of previous runs.
There is also a [documentation page](#).

A similar procedure has been recently developed, called the method of [Convolutional Multiple Whole Profile fitting](#), which is more sophisticated compared to the MWP method, so you should use the [CMWP method](#) when possible.

[MKDAT](#) is a program for preparing X-ray diffraction data for the [MWP program](#). The functions of the program: (i) stripping off background, (ii) separation of overlapping peaks and (iii) deconvolution of instrumental profiles. Follow [this](#) link to download it.

MWP output files:



Address <http://www.renyi.hu/cgi-bin/post-mwp-list>

MWP-fit: list of dragomir's samples

- [CeO2-1](#)
- [KiinduloMg](#)
- [KiinduloMg.fourier.dat](#)
- [KiinduloMg.fwhm.dat](#)
- [KiinduloMg.fwhm.tmp.dat](#)
- [KiinduloMg.int.dat](#)
- [KiinduloMg.intbr.dat](#)
- [KiinduloMg.sol](#)
- [MG](#)
- [Mg_as_rec](#)
- [ZrGr12](#)
- [ZrGr12a](#)
- [ZrGr2](#)
- [cuhpt50](#)
- [hptcu50](#)
- [prob](#)
- [zrgr12](#)
- [zrgr12AA](#)
- [zrgr12a](#)
- [zrgr12b](#)
- [zrgr12c](#)
- [zrgr12d](#)
- [zrgr12f](#)
- [zrgr13](#)
- [zrgr13a](#)
- [zrgr13b](#)
- [zrgr13c](#)
- [zrgr14](#)
- [zrgr14a](#)
- [zrgr14b](#)
- [zrgr15](#)
- [zrgr15a](#)

MWP output files:

.../comp.sol

The solutions:

a=-2.42784

b=3.18557

c=0.596521

d=291.947

e=0.0219218

m=exp(b)=24.1811

sigma=c/sqrt(2)=0.421804

D=41.4270197228895nm

d=33.8048nm

L0=25.1511nm

q=a=-2.42784

rho=2/(Pi*(0.382545nm*d)**2)=5.10396e-05(1/nm)^2

Re^*=exp(-1/4)/(2*e)=17.7632nm

M^*=(Re^*)*sqrt(rho)=0.126904

After 17 iterations the fit converged.

final sum of squares of residuals : 1.24613

rel. change during last iteration : 0

Final set of parameters

Asymptotic Standard Error

=====

=====

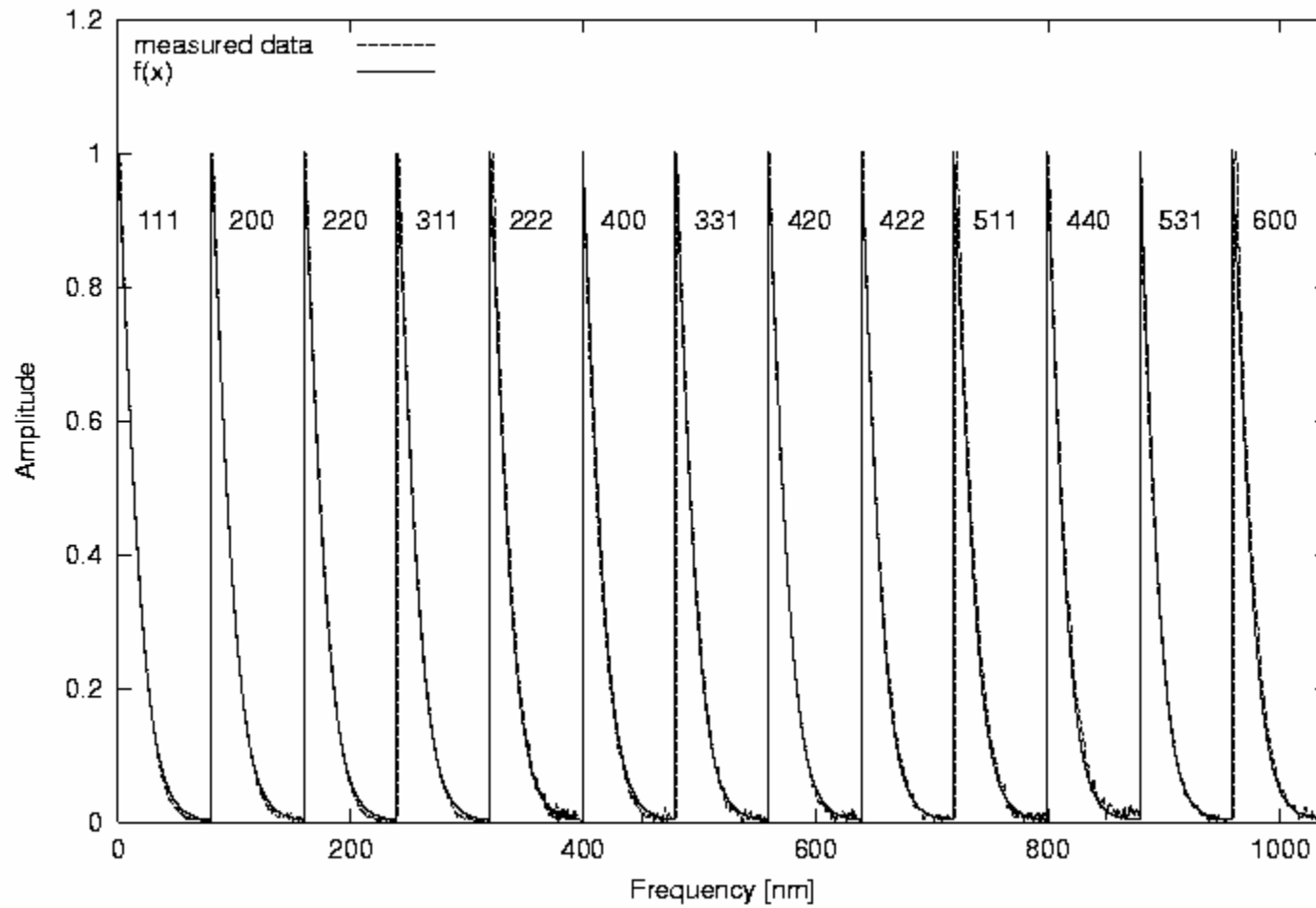
a	= -2.42784	+/- 0.3039	(12.52%)
b	= 3.18557	+/- 0.009763	(0.3065%)
c	= 0.596521	+/- 0.00484	(0.8114%)
d	= 291.947	+/- 7.676	(2.629%)

For more information about correlation matrix and confidence intervals, please read the file gatech/Ce02/S1/comp.fourier.sol.

*** END OF FITTING ***

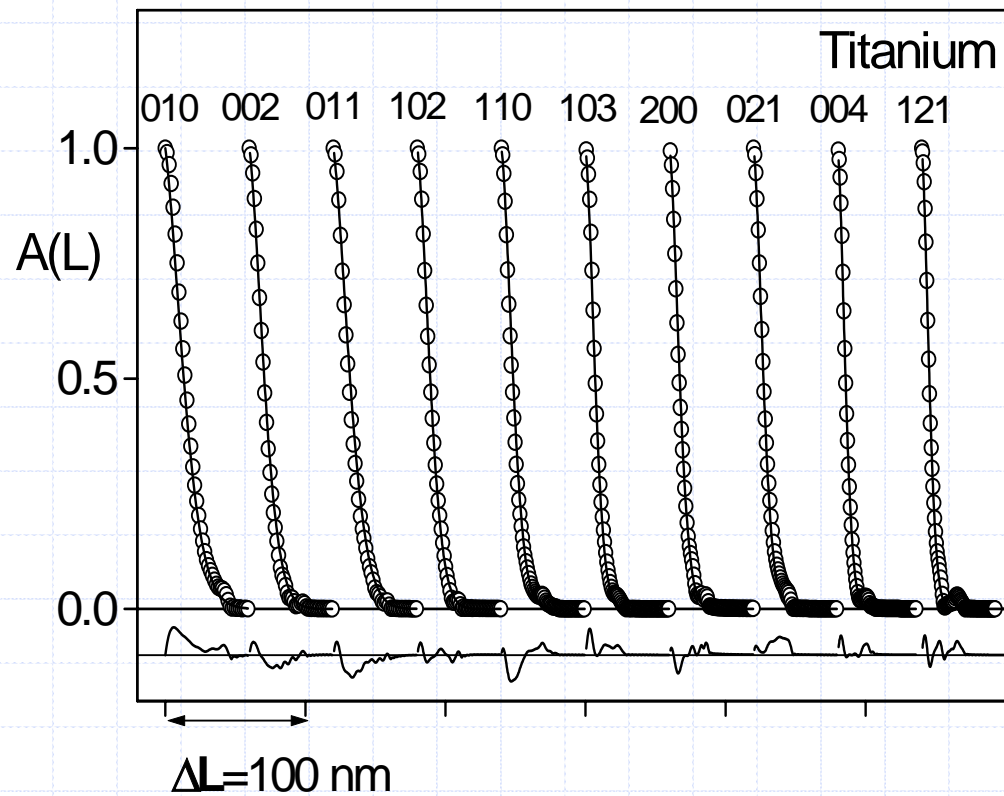
MWP output files:

.../S2MWP.Fourier.gif



MWP output files:

.../comp.fourier.th.dat & .../comp.fourier.m.dat



MWP References:

- Ungár, T., Gubicza, J., Ribárik, G. and Borbély, A.: Crystallite size-distribution and dislocation structure determined by diffraction profile analysis: principles and practical application to cubic and hexagonal crystals, *J. Appl. Cryst.* 34, 298-310, 2001
- Ribárik, G., Ungár, T. and Gubicza, J.: MWP-fit: a program for Multiple Whole Profile fitting of diffraction peak profiles by ab-initio theoretical functions, *J. Appl. Cryst.* 34, 669-676, 2001

CMWP - fit:

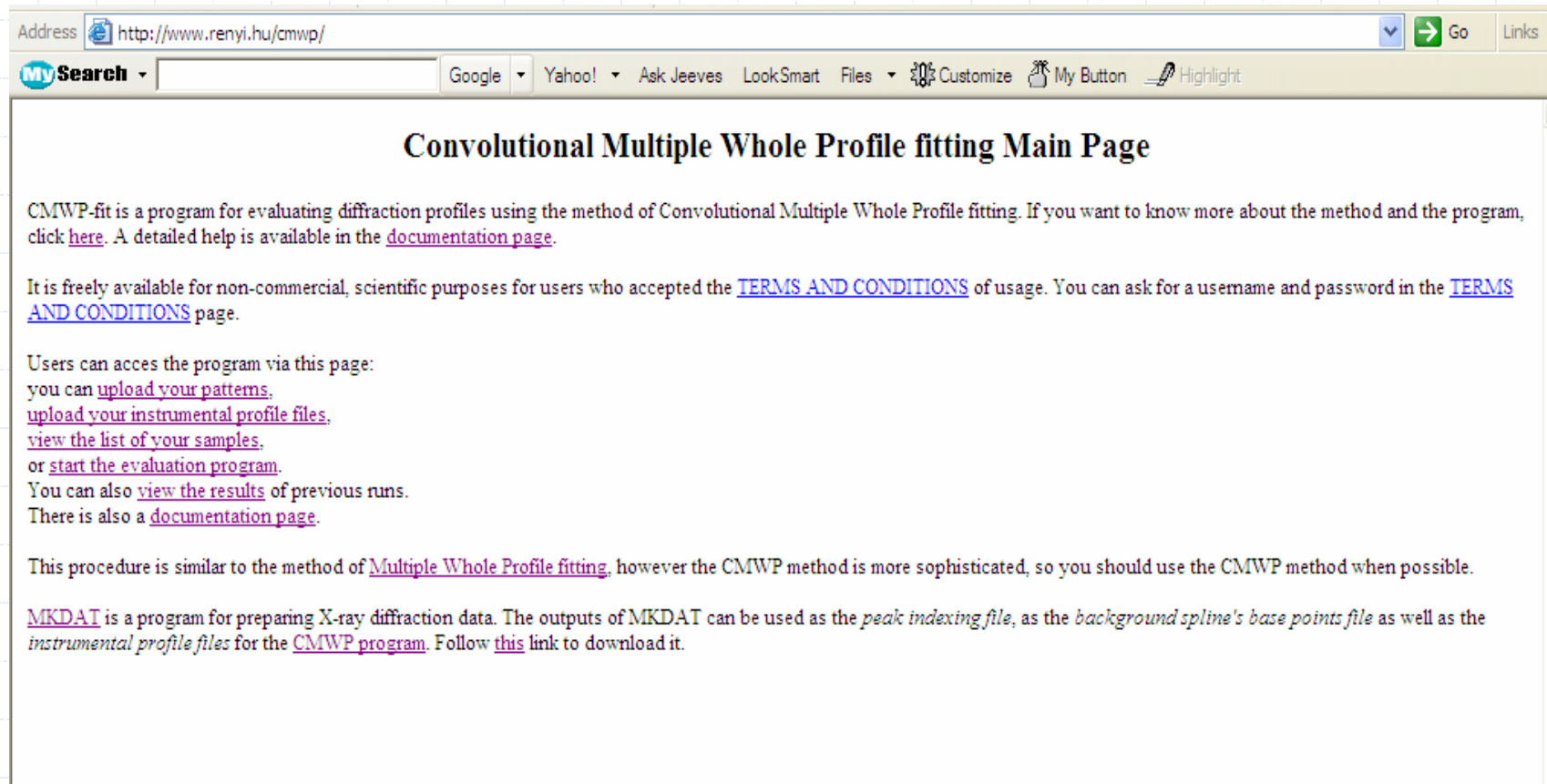
In order to avoid the uncertainties and the errors introduced by correction procedures in CMWP the measured pattern is directly fitted by the background plus the theoretical function of the pattern convoluted with the instrumental effect.

$$I_{theoretical} = BG(2\theta) + \sum_{hkl} I_{MAX}^{hkl} I^{hkl}(2\theta - 2\theta_0^{hkl}),$$

$$I^{hkl} = I_{instr.}^{hkl} * I_{size}^{hkl} * I_{dist.}^{hkl}$$

$$(I^{(meas)} - I^{(th)})^2 = \min. \quad \text{Nonlinear least squares method}$$

CMWP - fit:



The screenshot shows a web browser window with the address bar containing <http://www.renyi.hu/cmwp/>. The browser's search bar is set to "My Search" and includes links to Google, Yahoo!, Ask Jeeves, and LookSmart. The page title is "Convolutional Multiple Whole Profile fitting Main Page".

CMWP-fit is a program for evaluating diffraction profiles using the method of Convolutional Multiple Whole Profile fitting. If you want to know more about the method and the program, click [here](#). A detailed help is available in the [documentation page](#).

It is freely available for non-commercial, scientific purposes for users who accepted the [TERMS AND CONDITIONS](#) of usage. You can ask for a username and password in the [TERMS AND CONDITIONS](#) page.

Users can access the program via this page:
you can [upload your patterns](#),
[upload your instrumental profile files](#),
[view the list of your samples](#),
or [start the evaluation program](#).
You can also [view the results](#) of previous runs.
There is also a [documentation page](#).

This procedure is similar to the method of [Multiple Whole Profile fitting](#), however the CMWP method is more sophisticated, so you should use the CMWP method when possible.

[MKDAT](#) is a program for preparing X-ray diffraction data. The outputs of MKDAT can be used as the *peak indexing file*, as the *background spline's base points file* as well as the *instrumental profile files* for the [CMWP program](#). Follow [this link](#) to download it.

CMWP - fit – input files format:

1) measurement file - This is a two-column ASCII file. The first column should contain *Two Theta* and the second column contains the intensity values.

2) index file

2θ	I_{\max}	hkl
28.5943	5371.97	111
33.1285	1425.45	200
47.5281	2708.36	220
56.3854	2023.35	311
59.1299	381.12	222
69.4534	327.03	400
76.7388	703.47	331
79.1124	432.52	420
88.4608	577.85	422
95.4312	463.26	511
107.2531	117.04	440
114.7488	551.35	531
117.3341	250.49	600




3) background file




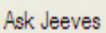
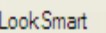

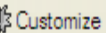
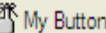
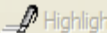
2θ	I
28.5943	118
33.1285	106
47.5281	95
56.3854	94
59.1299	94
69.4534	91
76.7388	89
79.1124	88
88.4608	88
95.4312	89
107.2531	93
114.7488	99
117.3341	100

4) instrumental profiles file

d^*	I/I_{\max}
-0.00394	0.203045
-0.0035	0.26193
-0.00306	0.330089
-0.00262	0.411947
-0.00219	0.515034
-0.00175	0.643361
-0.00131	0.757919
-0.00087	0.879088
-0.00044	0.978878
0	1
0.00044	0.96513
0.00088	0.867677
0.00131	0.730476
0.00175	0.583633
0.00219	0.437497
0.00263	0.313898
0.00306	0.219254
0.0035	0.148984
0.00394	0.0989103

CMWP - fit - upload:

Address  http://www.renyi.hu/cmwp/program/cmwp-upload.html  Go  Links >>

 My Search  Google  Yahoo!  Ask Jeeves  LookSmart  Files  Customize  My Button  Highlight

CMWP-fit Upload Page

Here you can transfer the powder pattern file, the indexing file and the background spline's base points file corresponding to your sample from your computer to your main directory with this simple tool. Specify the name of your sample (the basename of the files), click on the **Browse...** buttons to select the powder pattern file, the indexing file and the spline base points file and then click **Upload Files**.

Name of the sample:

Powder pattern file:

Indexing file:

Spline base points file:

Click [here](#) to start the evaluation procedure.

CMWP - fit:

Address http://www.renyi.hu/cmwp/program/cmwp-inst-upload.html Go Links >>

Mv Search Google Yahoo! Ask Jeeves LookSmart Files Customize My Button Highlight

CMWP-fit Instrumental Profile Upload Page

Here you can transfer the previously prepared instrumental profiles from your computer to your main directory with this simple tool. Note that these files should be two-column ASCII files, the first column should contain $K-K_0$ and the second contains the intensity values, where $K=2*\sin(\Theta)/\lambda$ and K_0 is the K value at the center of the peak. Specify the name of your instrumental sample (the name of the directory in which the instrumental profiles will be uploaded), specify the TwoTheta values in degrees, click on **Browse...** to select the files and then click **Upload Instrumental Profiles**.

Name of the instrumental sample:

TwoTheta:	<input type="text" value="30.385"/>	filename:	<input type="text" value="C:\work\denver\2005\MWP\CeO2\110"/>	<input type="button" value="Browse..."/>
TwoTheta:	<input type="text" value="37.44"/>	filename:	<input type="text" value="C:\work\denver\2005\MWP\CeO2\111"/>	<input type="button" value="Browse..."/>
TwoTheta:	<input type="text" value="43.51"/>	filename:	<input type="text" value="C:\work\denver\2005\MWP\CeO2\200"/>	<input type="button" value="Browse..."/>
TwoTheta:	<input type="text" value="48.957"/>	filename:	<input type="text" value="C:\work\denver\2005\MWP\CeO2\210"/>	<input type="button" value="Browse..."/>
TwoTheta:	<input type="text" value="53.99"/>	filename:	<input type="text" value="C:\work\denver\2005\MWP\CeO2\211"/>	<input type="button" value="Browse..."/>
TwoTheta:	<input type="text" value="63.22"/>	filename:	<input type="text" value="C:\work\denver\2005\MWP\CeO2\220"/>	<input type="button" value="Browse..."/>
TwoTheta:	<input type="text" value="67.55"/>	filename:	<input type="text" value="C:\work\denver\2005\MWP\CeO2\300"/>	<input type="button" value="Browse..."/>
TwoTheta:	<input type="text" value="71.745"/>	filename:	<input type="text" value="C:\work\denver\2005\MWP\CeO2\310"/>	<input type="button" value="Browse..."/>
TwoTheta:	<input type="text" value="75.84"/>	filename:	<input type="text" value="C:\work\denver\2005\MWP\CeO2\311"/>	<input type="button" value="Browse..."/>
TwoTheta:	<input type="text" value="79.87"/>	filename:	<input type="text" value="C:\work\denver\2005\MWP\CeO2\222"/>	<input type="button" value="Browse..."/>
TwoTheta:	<input type="text" value="83.85"/>	filename:	<input type="text" value="C:\work\denver\2005\MWP\CeO2\320"/>	<input type="button" value="Browse..."/>
TwoTheta:	<input type="text" value="87.79"/>	filename:	<input type="text" value="C:\work\denver\2005\MWP\CeO2\321"/>	<input type="button" value="Browse..."/>
TwoTheta:	<input type="text" value="95.67"/>	filename:	<input type="text" value="C:\work\denver\2005\MWP\CeO2\400"/>	<input type="button" value="Browse..."/>
TwoTheta:	<input type="text" value="99.64"/>	filename:	<input type="text" value="C:\work\denver\2005\MWP\CeO2\410"/>	<input type="button" value="Browse..."/>
TwoTheta:	<input type="text" value="103.66"/>	filename:	<input type="text" value="C:\work\denver\2005\MWP\CeO2\330"/>	<input type="button" value="Browse..."/>
TwoTheta:	<input type="text" value="107.75"/>	filename:	<input type="text" value="C:\work\denver\2005\MWP\CeO2\331"/>	<input type="button" value="Browse..."/>
TwoTheta:	<input type="text" value="111.93"/>	filename:	<input type="text" value="C:\work\denver\2005\MWP\CeO2\420"/>	<input type="button" value="Browse..."/>

Done Internet

CMWP - fit – crystal system:

The screenshot shows a Microsoft Internet Explorer browser window. The title bar reads "Convolutional Multiple Whole Profile fitting - Microsoft Internet Explorer". The address bar shows the URL "http://www.renyi.hu/cmwp/program/cmwp-run.html". The page content is on a light green background and includes the following sections:

- Evaluation of diffraction patterns using the method of Convolutional Multiple Whole Profile fitting**
- Files**
- A form field: "Please enter the name of the sample:
- Selection of the crystal system**
- A form field: "The crystal system is:" with two radio buttons: "cubic (default)" (selected) and "hexagonal".
- Input parameters**

The browser's status bar at the bottom shows "Done" and "Internet".

CMWP - fit – input parameters:

Convolucional Multiple Whole Profile fitting - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address <http://www.renyi.hu/cmwp/program/cmwp-run.html> Go Links >>

Search Google Yahoo! Ask Jeeves LookSmart Files Customize My Button Highlight

cubic (défaut)
hexagonal

Input parameters

Please enter the value of the lattice constant "a" (in nm):

Please enter the value of the lattice constant "c" (in nm):

Please enter the value of the absolute value of the Burgers vector (in nm):

Please enter the average contrast factor of the h00 (or hk0) reflections:

Please enter the wavelength (in nm):

Please note that setting of the lattice parameter "c" has effect only if the crystal system is hexagonal.

Instrumental profiles

Set this if you have instrumental profiles:

If you have instrumental profiles, please enter the name of the of the instrumental profile directory:

The interval used for fitting and plotting

The interval used for fitting and plotting is: [minx,maxx]

Done Internet

CMWP - fit - fitting interval:

Convolutional Multiple Whole Profile fitting - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address <http://www.renyi.hu/cmwp/program/cmwp-run.html>

my Search Google Yahoo! Ask Jeeves LookSmart Files Customize My Button Highlight

If you have instrumental profiles, please enter the name of the of the instrumental profile directory:

The interval used for fitting and plotting

The interval used for fitting and plotting is: [minx,maxx]

Please specify the value of minx (in degrees):

Please specify the value of maxx (in degrees):

Please note that if you don't fill these fields, all the data in the measured powder pattern file will be used.

Selection of the size function

The program will use the spheric size function (default)

The program will use the ellipsoidal size function

The program will disable the size effect

CMWP - fit – settings/initial values:

Sampling of the simulated powder pattern data

Please specify N1:

Please specify N2:

Please specify the profile cutting parameter (in Two theta degrees):

Initial values of the parameters

Please enter the initial value of the parameter "a" (or "a1"): fix:

Please enter the initial value of the parameter "a2": fix:

Please enter the initial value of the parameter "b": fix:

Please enter the initial value of the parameter "c": fix:

Please enter the initial value of the parameter "d": fix:

Please enter the initial value of the parameter "e": fix:

Please enter the initial value of the parameter "epsilon": fix:

fix d*e:

Please note that setting of the parameter "a2" has effect only if the crystal system is hexagonal and setting of the parameter "epsilon" has effect only if the size function is ellipsoidal.

Done

Internet

CMWP - fit – refinement/fit control:

Peak parameter refinement and weighting

Set this if you want to fit the peak positions and peak intensities:

Set this if you want to use weights in the fitting algorithm:

Fit control


Please specify the limit for stopping:

Please specify the maximal number of iterations:

After filling in the relevant fields in this form, please press/click this button: to begin the evaluation procedure. Click the button to reset the values.

CMWP - fit –fitting.....:






Address  http://www.renyi.hu/cgi-bin/post-cmwp?SAMPLENAME=CeO2-S1&HEXAGONAL_CRYSTAL=n&la=0.541&lc=0&bb=0.32&C0=0.3&wavelength=0.154&have_ir

Convolutional Multiple Whole Profile fitting

Connecting the server for evaluation
The evaluation is started.
Please wait until this page loads to get the results.

Note that the results will be stored in <http://www.renyi.hu/cmwp/results/dragomir/CeO2-S1-2005-08-02-07-03-55>.

Address  http://www.renyi.hu/cgi-bin/post-cmwp?SAMPLENAME=CeO2-S1&HEXAGONAL_CRYSTAL=n&la=0.541&c=0&bb=0.32&CO=0.3&wavelength=0.154&have_inst_prof   G

Convolutional Multiple Whole Profile fitting

Connecting the server for evaluation
The evaluation is started.
Please wait until this page loads to get the results.

Note that the results will be stored in <http://www.renyi.hu/cmwp/results/dragomir/CeO2-S1-2005-08-02-07-03-55>.

The fitting is done, evaluate's output follows:

This is CMWP-fit, a program for evaluation of diffraction patterns using the method of Convolutional Multiple Whole Profile fitting. Copyright (C) Gábor Ribárik, 1998-2004. All rights reserved. For permission to use, copy, modify this program or any of its components, ask the authors. Redistributing this software is not allowed.


Date: 2005-08-02 07:04:00

Data file: dragomir/CeO2-S1/CeO2-S1.dat

The value of the lattice constant (in nm): 0.541
The absolute value of the Burgers vector (in nm): 0.32
The average contrast factor of the h00 reflections: 0.3
The wavelength is: 0.154 nm.
The definition of the Size Function:
$$sf_spheric(k,b,c)=\text{Int}(0.5*x*\text{erfc}((\log(x)-b)/c)*(\sin(\text{Pi}*k*x)/(\text{Pi}*k))^{**2},x=0..Inf)$$

Found peak at 28.5943, intensity: 5371.97.
hkl=111
H2=0.333333
g^2=10.2501



Address  http://www.renyi.hu/cgi-bin/post-cmwp?SAMPLENAME=CeO2-S1&HEXAGONAL_CRYSTAL=n&a=0.541&c=0&bb=0.32&C0=0.3&wav

11_11_2024
*** FIT ***

Calculating a,b,c,d,e to fit the measured powder diffraction pattern
with the corresponding theoretical function.

The initial values of the parameters:

C0=0.3

a = 1

b = 3

c = 1

d = 80

e = 0.05

epsilon = 1.0 # FIXED

The solutions:

a=0.288428

b=3.17207

c=0.59686

d=13.858

e=18.7037

m=exp(b)=23.8568

sigma=c/sqrt(2)=0.422044

D=gnuplot>nm

d=33.3751nm

L0=24.8264nm

q=a=0.288428

rho=2/(Pi*(0.32nm*d)**2)=0.0323727(1/nm)^2

Re^*=exp(-1/4)/(2*e)=0.0208194nm

M^*=(Re^*)*sqrt(rho)=0.00374591

After 334 iterations the fit converged.

final sum of squares of residuals : 5.84622e+06

rel. change during last iteration : -9.99023e-10

Final set of parameters


Asymptotic Standard Error

=====

=====

a	= 0.288428	+/- 0.1331	(46.15%)
---	------------	------------	----------



Address  http://www.renyi.hu/cgi-bin/post-cmwp?SAMPLENAME=CeO2-S1&HEXAGONAL_CRYSTAL=n&a=0.541&c=0&bb=0.32&CO=0.3&wavelength=0.1

The solutions:

a=0.288428
b=3.17207
c=0.59686
d=13.858
e=18.7037

m=exp(b)=23.8568
sigma=c/sqrt(2)=0.422044
D=gnuplot>nm
d=33.3751nm
L0=24.8264nm

q=a=0.288428
rho=2/(Pi*(0.32nm*d)**2)=0.0323727(1/nm)^2
Re**=exp(-1/4)/(2*e)=0.0208194nm
M**=(Re**)*sqrt(rho)=0.00374591

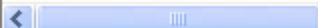
After 334 iterations the fit converged.

final sum of squares of residuals : 5.84622e+06
rel. change during last iteration : -9.99023e-10

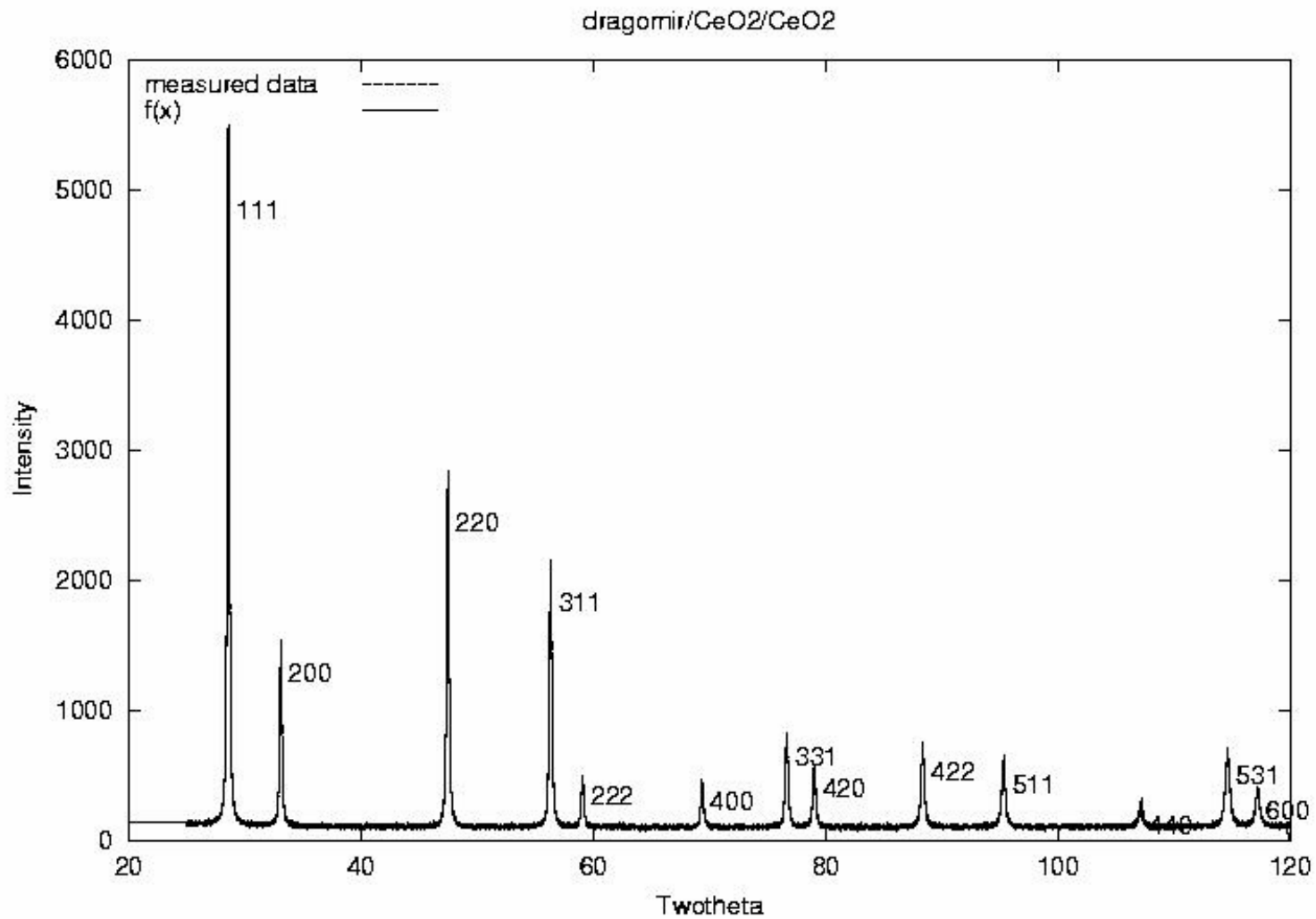
Final set of parameters	Asymptotic Standard Error
=====	=====
a = 0.288428	+/- 0.1331 (46.15%)
b = 3.17207	+/- 0.004389 (0.1384%)
c = 0.59686	+/- 0.001963 (0.3288%)
d = 13.858	+/- 48.26 (348.3%)
e = 18.7037	+/- 130.5 (697.9%)

For more information about correlation matrix and confidence intervals,
please read the file dragomir/CeO2-S1/CeO2-S1.int.sol.

*** END OF FITTING ***



CMWP procedure - output:



CMWP References:

G. Ribárik, J. Gubicza, T. Ungár: Correlation between strength and microstructure of ball milled Al-Mg alloys determined by X-ray diffraction, Mater. Sci. Eng. A 387-389 (2004) 343-347.

Common features:

- Both procedures uses the *whole X-ray diffraction pattern*.
- The diffraction profiles are fitted by well established size and strain *physical* profile functions.

Differences:

- MWP fits all at once the Fourier transforms or the inverse Fourier transforms of the measured profiles after they were corrected for instrumental effect and background.
- CMWP fits the whole pattern with the convolution of the physical profiles and the instrumental effect plus the background.

Microstructural parameters obtained from MWP and CMWP procedures:

Cubic crystal systems:

m, σ : → size profile
 q : → strain anisotropy
 ρ^*, M → strain profile

Hexagonal crystal systems:

m, σ → size profile
 q_1 and q_2 → strain anisotropy
 ρ^*, M → strain profile

Theoretical individual and average contrast factor of dislocations

Or can be calculated using ANIZC software at <http://metal.elte.hu/anizc/>



AnizC program was developed by Dr. Andras Borbely (Department of General Physics at Eotvos Science University in Budapest, Hungary).

Reference: Borbely A., Dragomir-Cernatescu I., Ribárik G. and Ungár T.: "Computer program ANIZC for the calculation of diffraction contrast factors of dislocations in elastically anisotropic cubic, hexagonal and trigonal crystals", in J. Appl. Cryst., 36, 160-162, (2003)

Theoretical individual and average contrast factor of dislocations

AnizC for cubic crystals

Address <http://metal.elte.hu/anizc/program-cubic.html>

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Cubic lattices

Input* : C or S

C ₁₁	C ₁₂	C ₄₄
or	or	or
S ₁₁ *	S ₁₂ *	S ₄₄ *
<input type="text"/>	<input type="text"/>	<input type="text"/>

lg* :

The program computes* :

the individual contrast factor for a single dislocation:

b:	n:	l:
<input type="text"/>	<input type="text"/>	<input type="text"/>

or the average contrast factor for:

- edge <110>{111} type dislocations
- edge <111>{110} type dislocations
- edge <111>{211} type dislocations
- screw <110> type dislocations
- screw <111> type dislocations

Done

Theoretical individual and average contrast factor of dislocations

AnizC for hexagonal crystals

Address <http://metal.elte.hu/anizc/program-hexagonal.html>

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The Program Anizc

Input : C or S

C ₁₁ or S ₁₁ *	C ₁₂ or S ₁₂ *	C ₄₄ or S ₄₄ *
<input type="text"/>	<input type="text"/>	<input type="text"/>
C ₁₃ or S ₁₃ *	C ₃₃ or S ₃₃ *	c/a *
<input type="text"/>	<input type="text"/>	<input type="text"/>

g * :

The program computes * :

the individual contrast factor for a single dislocation:

b :	n :	l :
<input type="text"/>	<input type="text"/>	<input type="text"/>

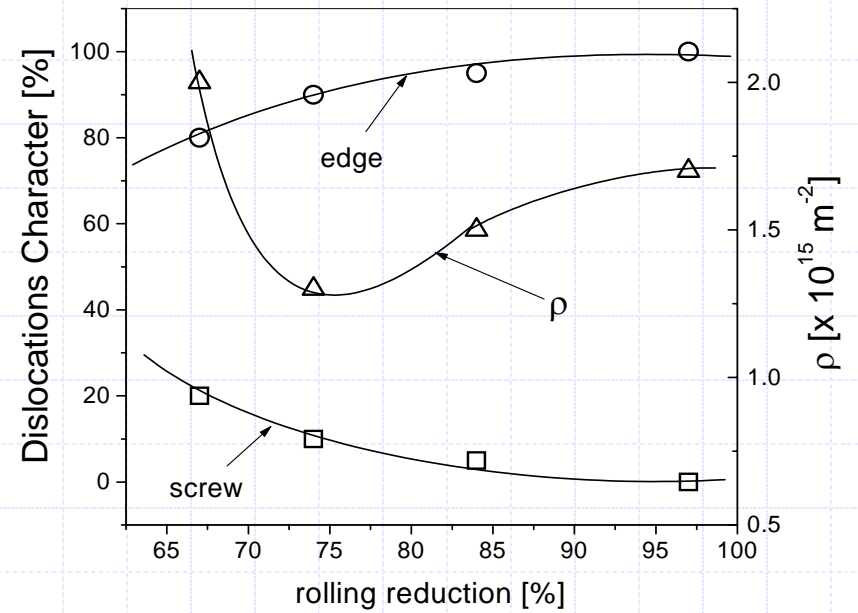
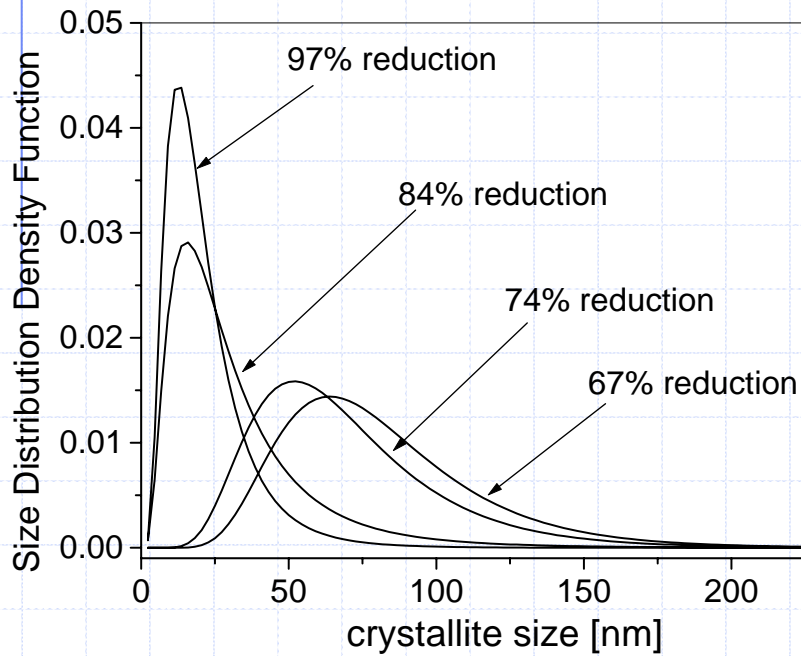
or the average contrast factor for:

- edge <-12-10>{10-10} type dislocations
- edge <-12-10>{10-11} type dislocations
- edge <-2110>{0001} type dislocations
- edge <-2113>{01-10} type dislocations

Done

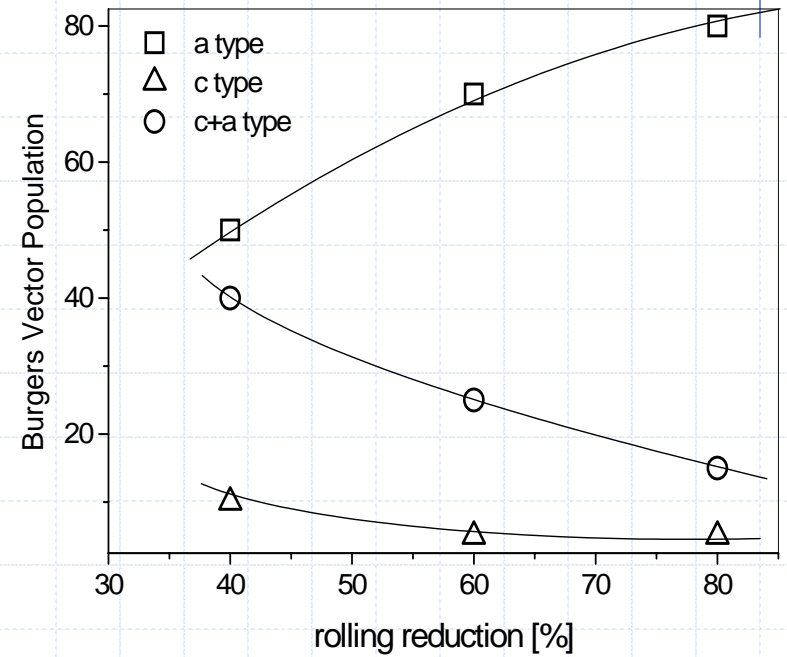
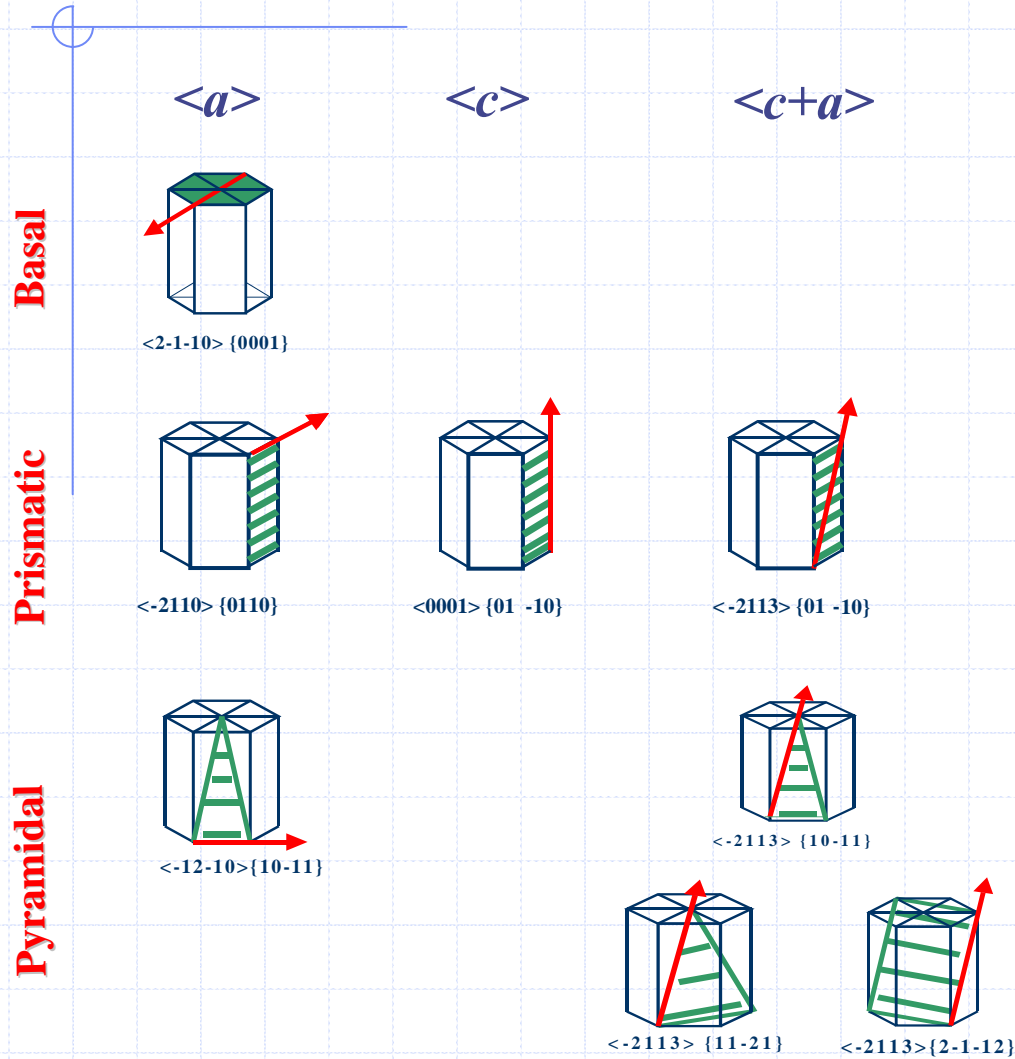
Applications:

Crystallite size distribution and Dislocation density and type in **nano-Cu** as a function of deformation



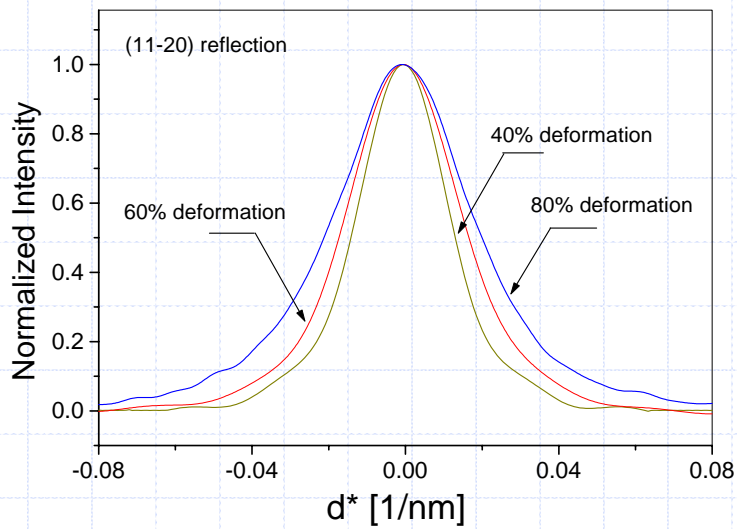
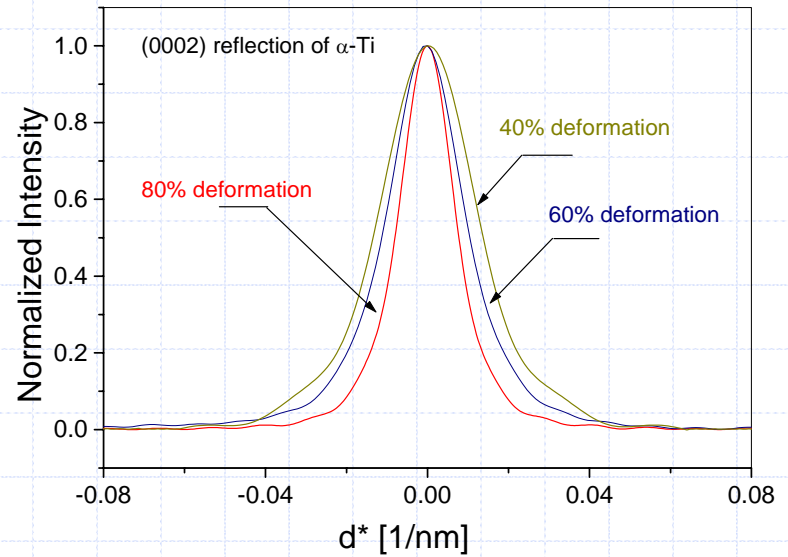
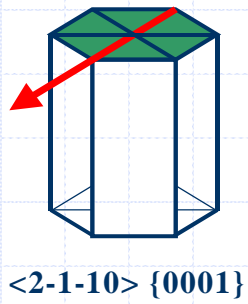
Applications:

Burgers vector types in Titanium deformed by rolling at 500^o F



Applications:

Burgers vector types in Titanium deformed by rolling at 500° F



Summary

MWP or CMWP procedure enables the determination of the sample microstructure from the X-ray diffraction pattern in terms of:

- 1) crystallite size distribution
- 2) dislocation density
- 3) dislocations type
- 4) dislocations arrangement.

Acknowledgements are due to *Prof. Ungar Tamas* and *Dr. Ribarik Gabor* for continuous help provided in the preparation of the present tutorial.