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

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54th Annual Denver X-ray Conference 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 (Multiple Whole Profile Fitting),
- 5) CMWP (Convolutional Multiple Whole Profile Fitting),
- 6) ANIZC program,
- 7) Examples,
- 8) Summary.

MWP and CMWP-fit

MWP and **CMWP**-fit are computer programs developed by <u>*Prof. Ungar*</u> <u>*Tamas*</u> and <u>*Dr. Ribarik Gabor*</u> (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)

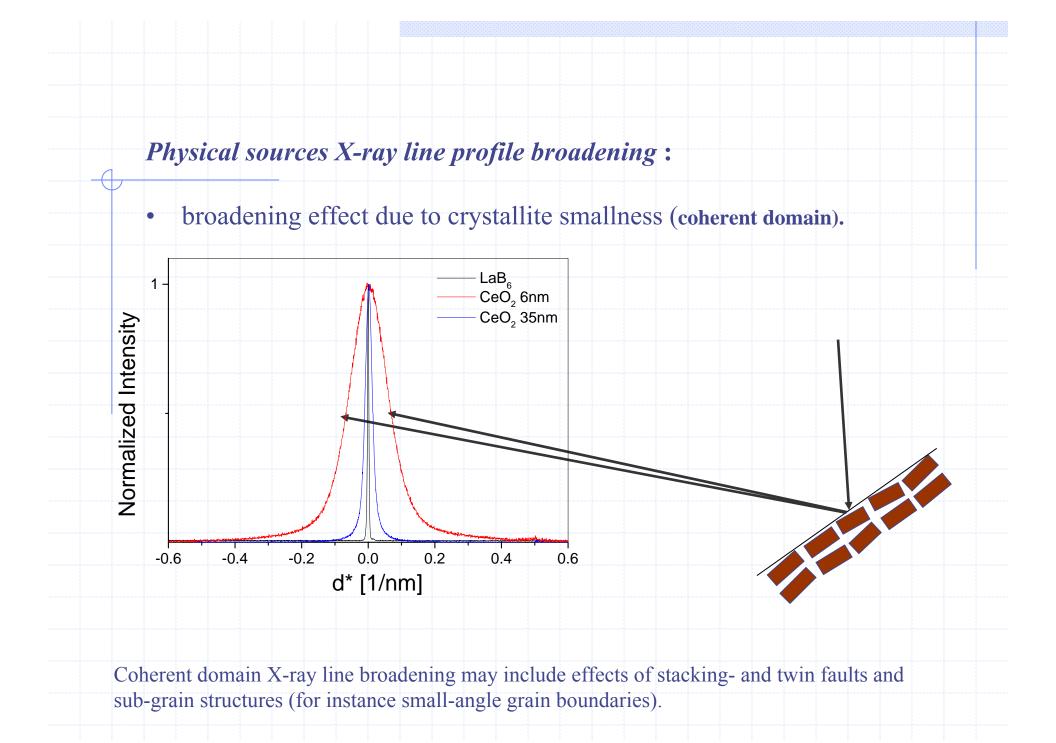


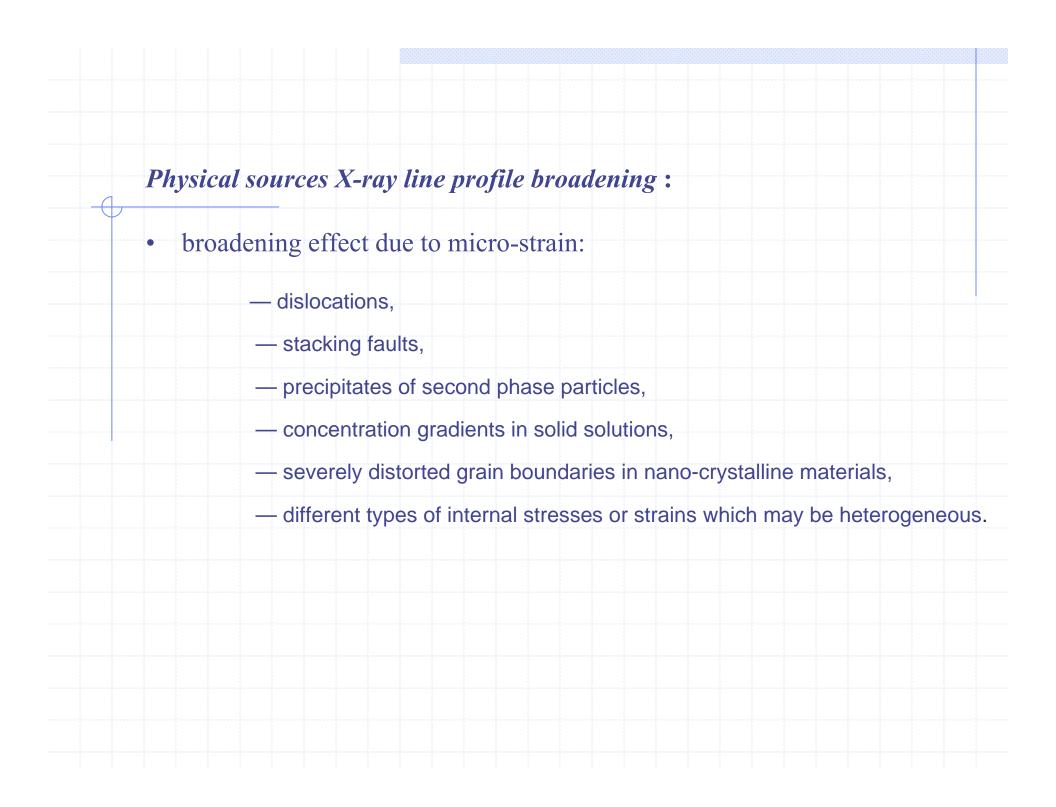


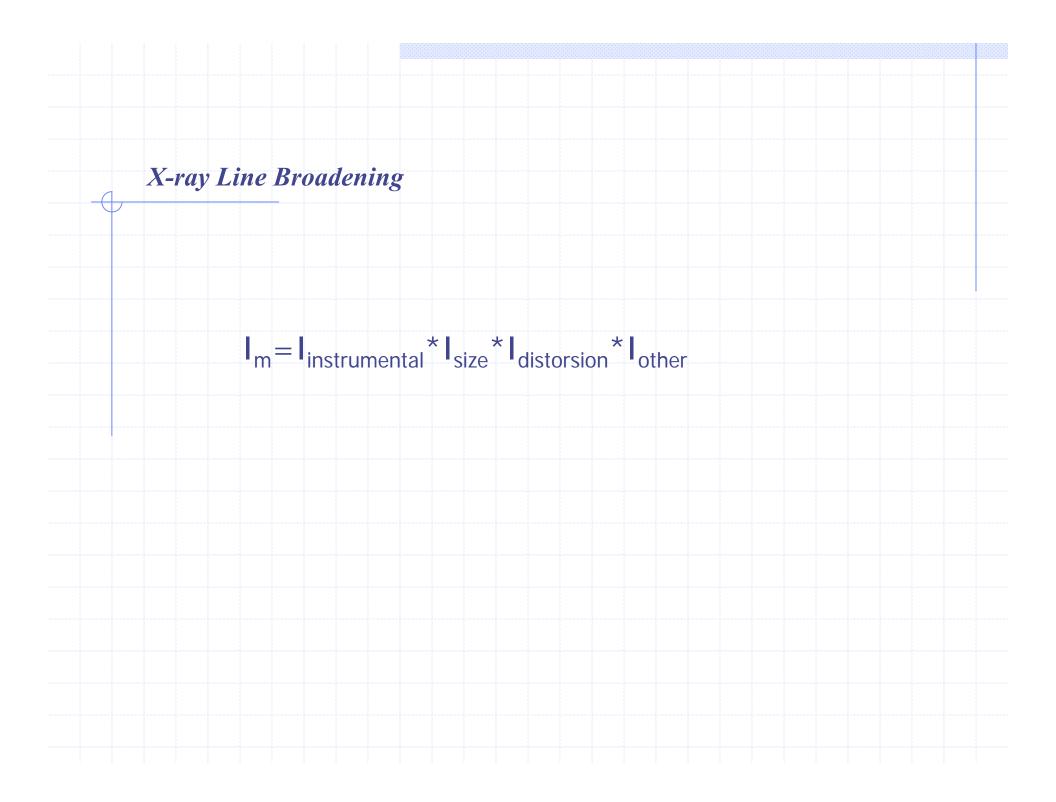




Standards for instrumental broadening: SRM660a (LaB₆), SRM640c (Si) - NIST
Standard specimen preparation: Berkum, J. G. M. van, Sprong, G. J. M., Keijser, Th. H. de, Delhez, R. and
Sonneveld, E. J. (1995), Powder Diffr. 10, 129-139







MWP and CMWP-fit - theoretical background

Assumptions:

- 1) X-ray diffraction line is broadened due to:
 - small coherent domains (usually smaller then 1 μ 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 - $I_m = I_{size} * I_{distorsion}$

Size effect:

Assumption \rightarrow log-normal size distribution and spherical crystallites:

$$I_{size}(s) = \int_{0}^{\infty} \mu \, \frac{\sin^2(\mu \, \pi s)}{(\pi s)^2} \, \text{erfc} \left[\frac{\log\left(\frac{\mu}{m}\right)}{\sqrt{2}\sigma} \right] \, \mathrm{d}\mu$$

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 - $I_m = I_{size} * I_{distorsion}$

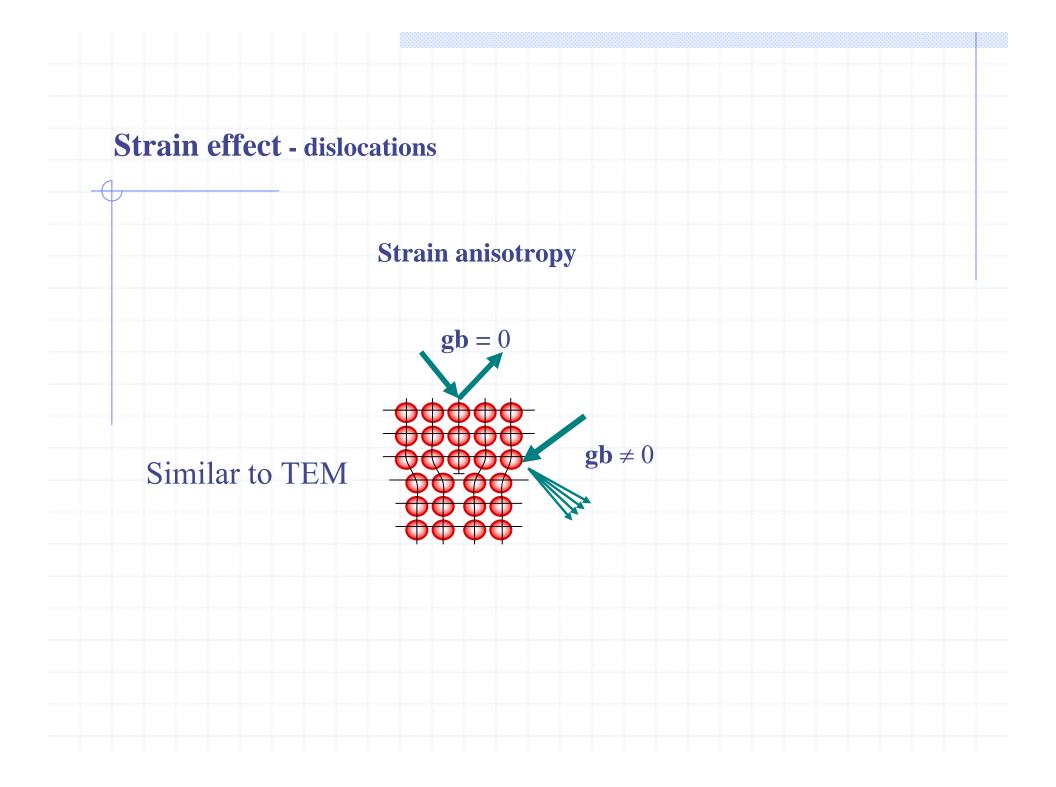
$$A(L) = A^{size}(L) A^{distorsion}(L)$$

Strain effect - dislocations:

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

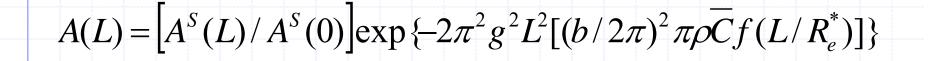
$A^{D}(L) = \exp\{-2\pi^{2}g^{2}L^{2}[(b/2\pi)^{2}\pi\rho\overline{C}f(L/R_{e}^{*})]\}$

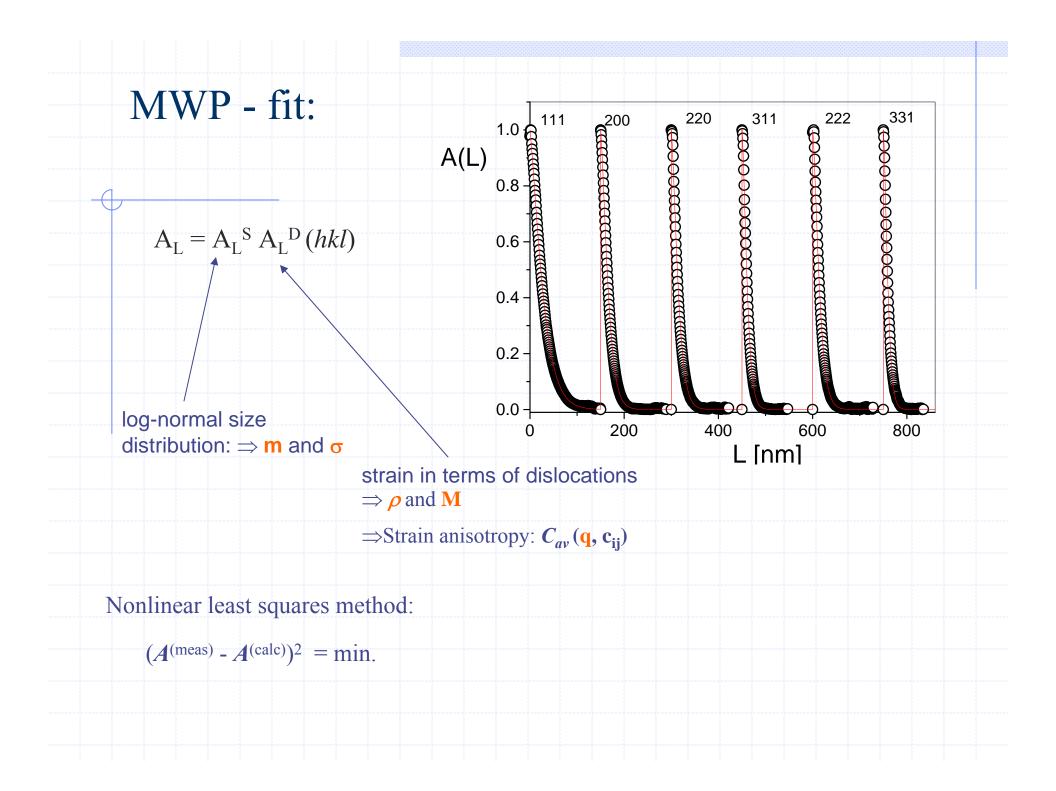
where g is the absolute value of the diffraction vector; L is the Fourier length, b is the absolute value of the Burgers vector, ρ is the dislocation density; \overline{C} is the average contrast factor of dislocation; R_e^* is the effective outer cut-off radius and f is the Wilkens function.





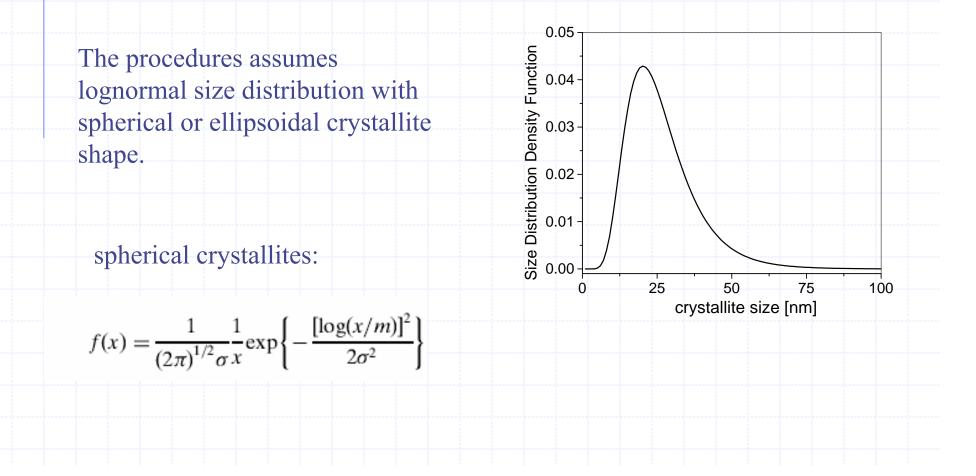
The Fourier transforms of the measured profiles are fitted all at once with:





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

Crystallite size distribution:



Strain anisotropy parameter, q :

Average contrast factors of dislocations for cubic crystal systems:

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

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

q depends on the a) studied material elastic proprieties,

b) dislocation geometry/character.

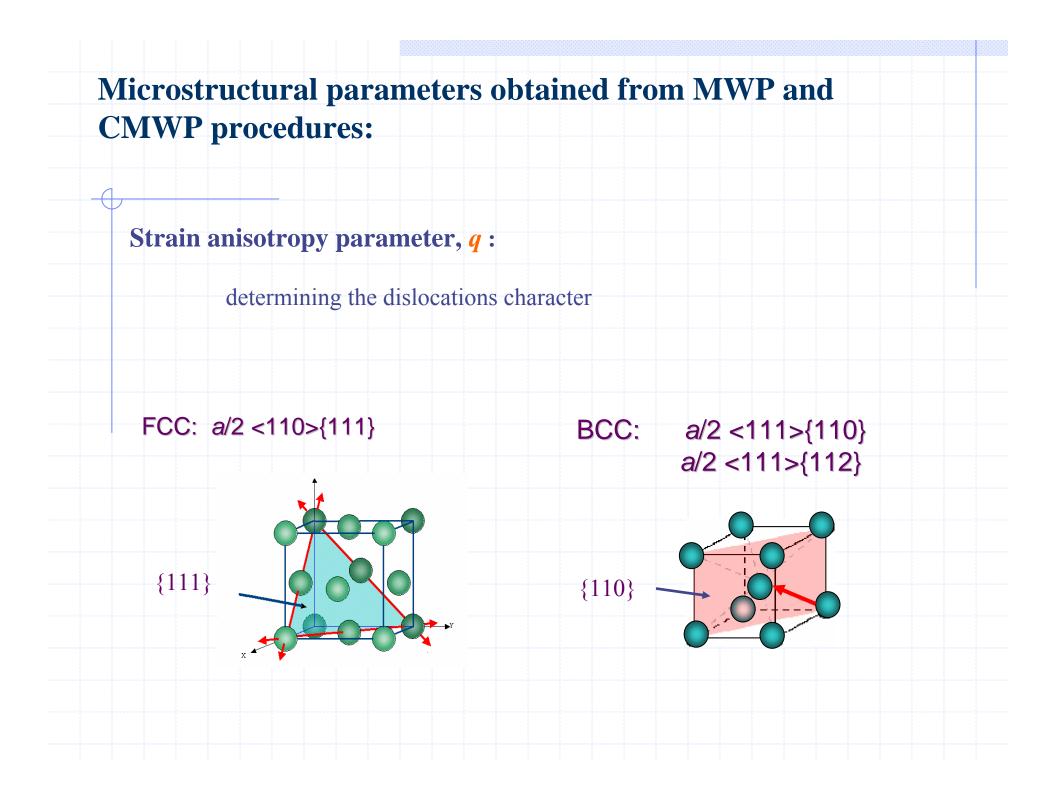
Reference: Ungár, T., Tichy, G. The effect of dislocation contrast on X-ray line profiles in untextured polycrystals. Phys. Stat. Sol. 1999;171:425434.

Microstructural parameters obtained from MWP and CMWP procedures:

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

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.



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

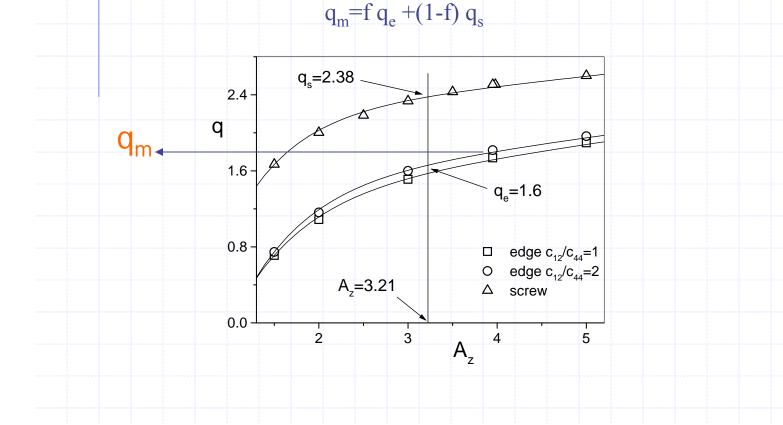
Ungár, T., Dragomir, I., Révész, Á., and Borbély, A.: "The Contrast Factors of Dislocations in Cubic Crystals: the Dislocation Model of Strain Anisotropy in Practice", J. Appl. Cryst., 32, 992-1002, (1999).

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).

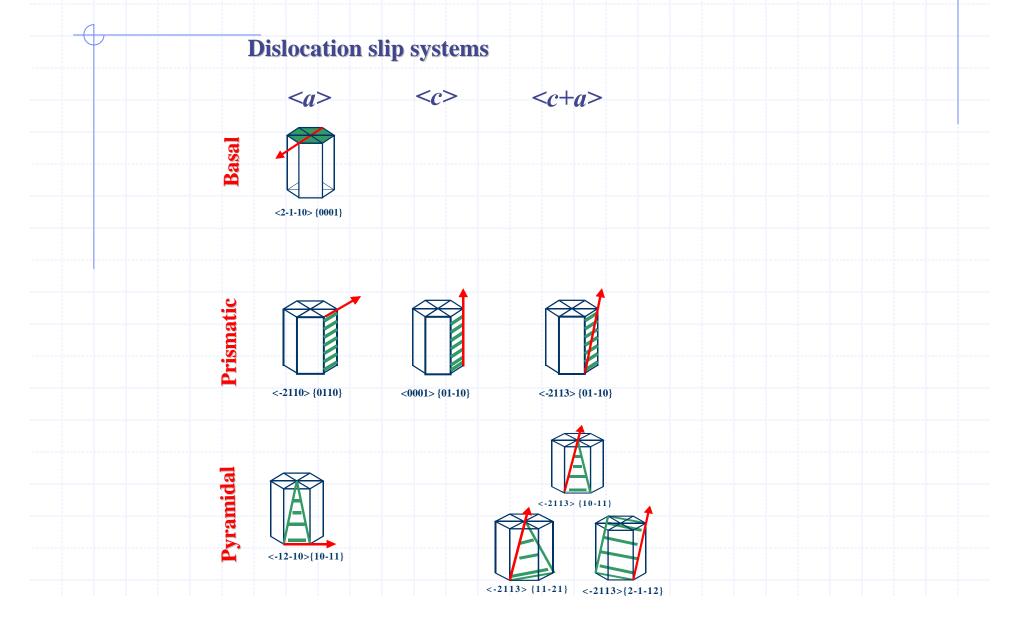
Microstructural parameters obtained from MWP and CMWP procedures:

Cubic crystal systems – theoretical average dialocation contrast factor:

FCC system - dislocation slip systems: 1/2<110>{111} type



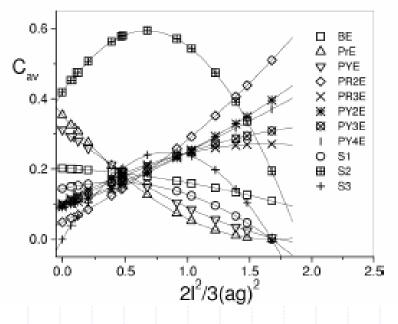
Average dislocation contrast factor for hexagonal crystal systems:



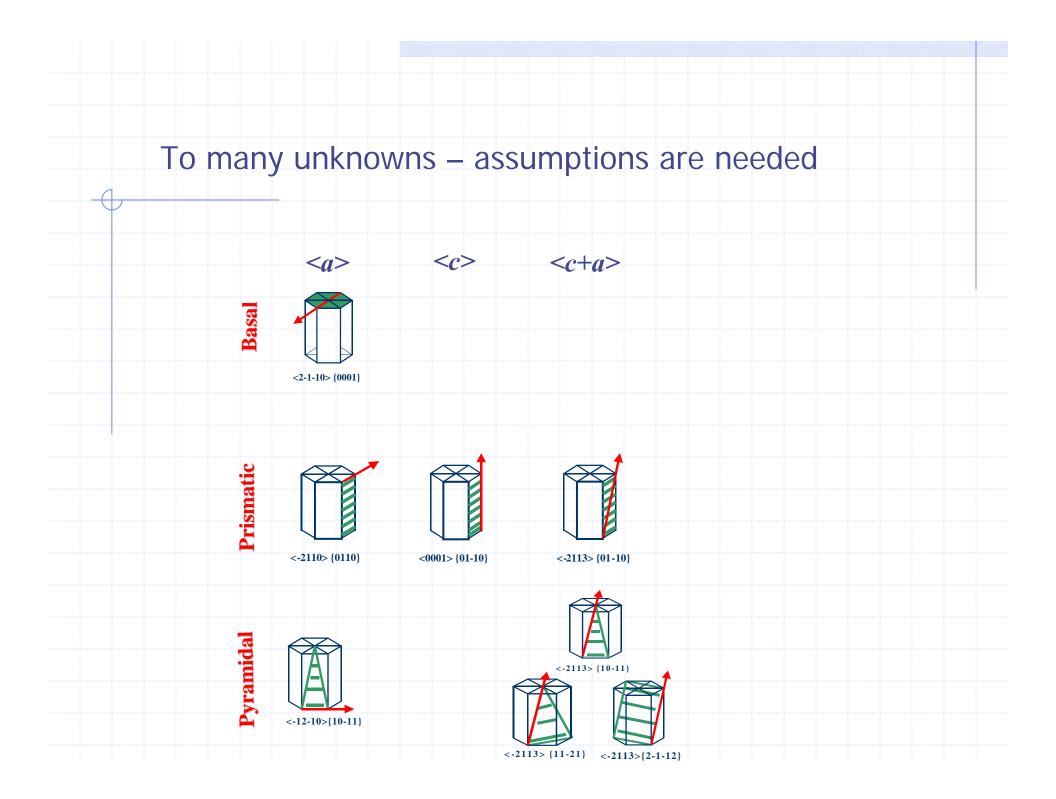
Microstructural parameters obtained from MWP and CMWP procedures:

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

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



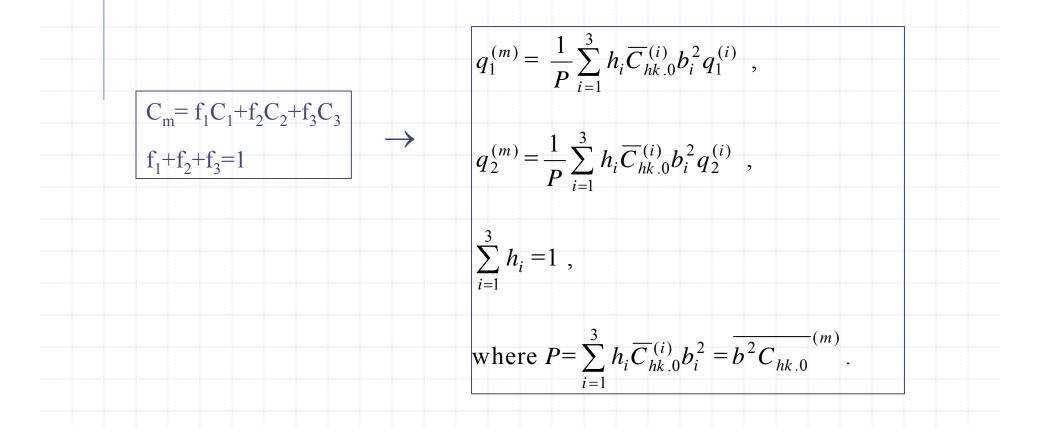
Dragomir I. C. and Ungár T.: "The contrast factors of dislocations in the hexagonal crystal system" in J. Appl. Cryst., 35, 556-564, (2002).



Microstructural parameters obtained from MWP and CMWP procedures:

Hexagonal crystal systems, q_1 and q_2 :

Measured and Theoretical average contrast factor of dislocations:



Microstructural parameters obtained from MWP and CMWP procedures – dislocation density

Evaluation of real dislocation density, ρ :

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

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

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

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

Microstructural parameters obtained from MWP and CMWP procedures – arrangement parameter

Dislocation arrangement parameter, *M* (Wilkens, 1970):

M is defined by Wilkens as the dislocation arrangement parameter.

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

M >> 1 week screening of dislocations fields

M ~ 1 quasi-homogeneous dislocation arrangement

M << 1 strong screening of dislocations filed, dipole configurations

MWP-fit:

Before using MWP the following profile corrections are necessary:

i) background
ii) overlapping peaks
iii) Kα₂
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:

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MWP - fit - Input files

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	-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:

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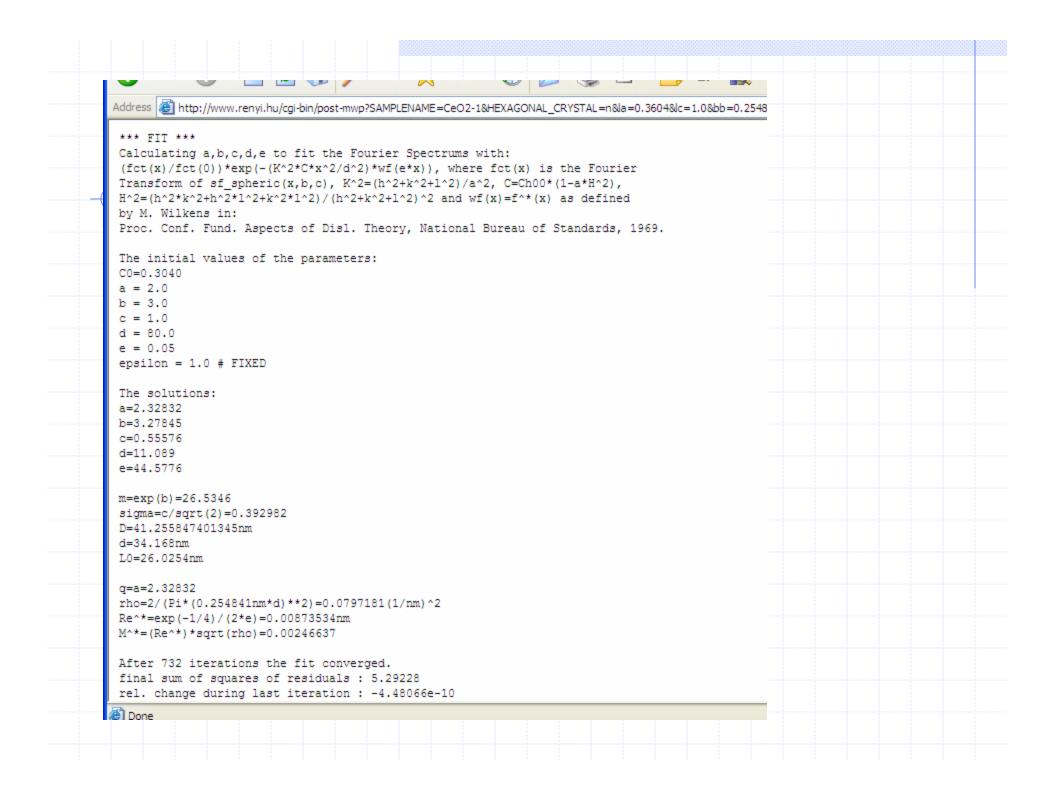
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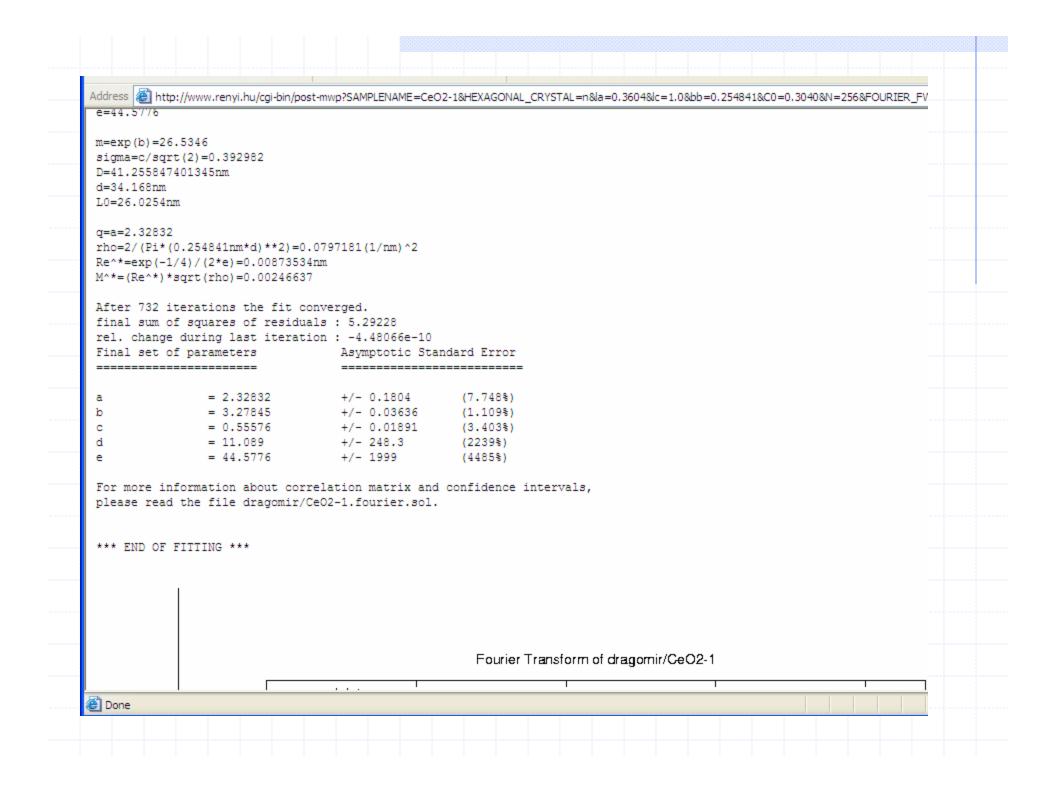
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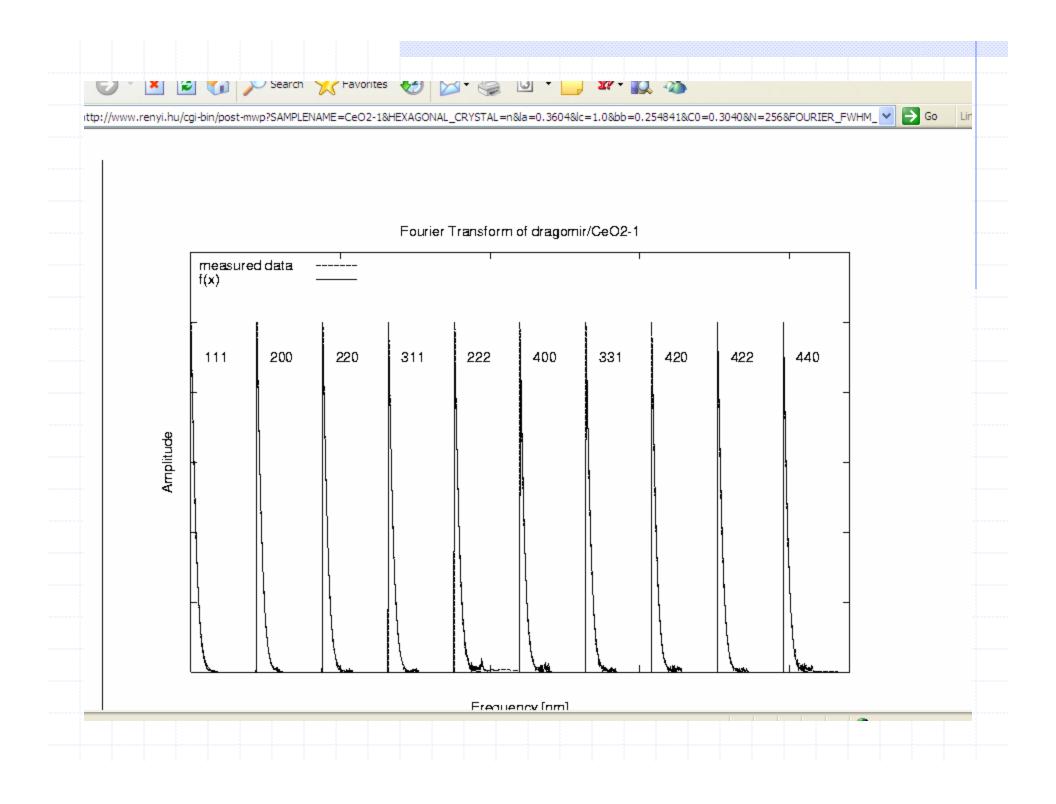
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		Multiple Wh	ole Profile fi	itting	
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Connecting the server for ev	aluation				
The evaluation is started. Please wait until this page lo	ads to get the results.				
Note that the results will be	stored in <u>http://www.renyi.r</u>	uu/mwp/results/dragomir/CeO	2-1-2005-08-02-05-46-33.		
The fitting is done, evaluate	s output follows:				
theoretical line profi Copyright (C) Gábor Ri	le functions. bárik and Tamás Ungá: copy, modify this p:	ole Profile Fitting usi r, 1998-2000. All right rogram or any of its co are is not allowed.	s reserved.		
Date: 2005-08-02 05:40	:34				
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*** FIT ***					







Search Coogle Yahoo! Ask Jeeves LookSmat Files W Customize My Button Highlight KUP-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, clice tetailed help is available in the documentation page. t 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 AND CONDITIONS page. Jsers can access the program via this page: You can upload your profile files. You can upload your profile files. You can also view the results of previous runs. Chere is also a documentation page.
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similar procedure has been recently developed, called the method of Convolutional Multiple Whole Profile fitting, which is more sophisticated compared to the MWP met
ould use the <u>CMWP method</u> when possible.
KDAT 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 per
convolution of instrumental profiles. Follow <u>this</u> link to download it.

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

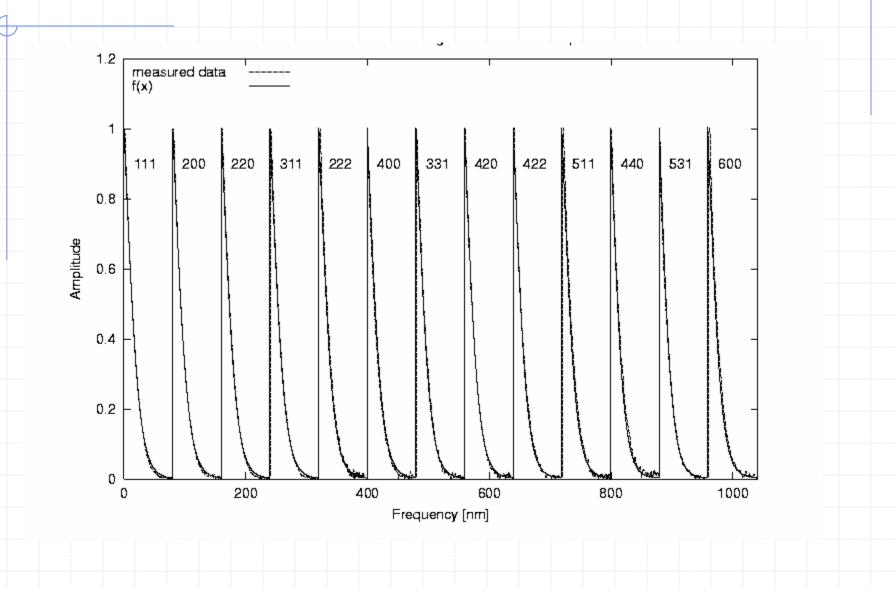
zrgr13a zrgr13b zrgr13c zrgr14 zrgr14a zrgr14b zrgr15 zrgr15a

.../comp.sol

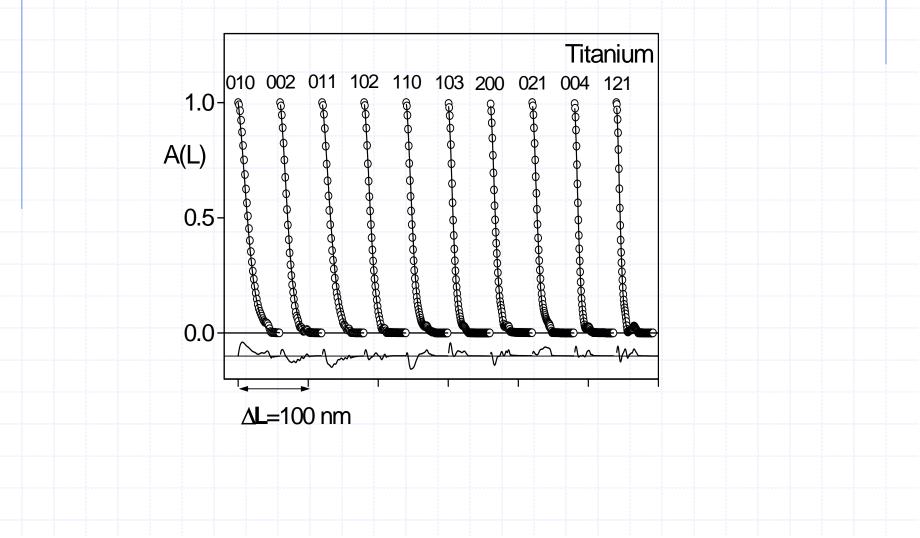
The solutions: a = -2.42784b=3.18557 c=0.596521 d=291.947 e=0.0219218 $m = \exp(b) = 24.1811$ sigma=c/sqrt(2)=0.421804 D=41.4270197228895nm d=33.8048nm L0=25.1511nm q=a=-2.42784 rho=2/(Pi*(0.382545nm*d)**2)=5.10396e-05(1/nm)^2 Re^*=exp(-1/4)/(2*e)=17.7632nm M^*=(Re^*)*sqrt(rho)=0.126904 After 17 iterations the fit converged. final sum of squares of residuals : 1.24613 rel. change during last iteration : 0 Final set of parameters Asymptotic Standard Error _____ _____ = -2.42784+/- 0.3039 (12.52%)а b = 3.18557 +/- 0.009763(0.3065%)= 0.596521+/- 0.00484(0.8114%)С (2.629%) d = 291.947+/- 7.676 For more information about correlation matrix and confidence intervals, please read the file gatech/CeO2/S1/comp.fourier.sol.

*** END OF FITTING ***

.../S2MWP.Fourier.gif



.../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.

$$I_{theoretical} = BG(2\Theta) + \sum_{hkl} I_{MAX}^{hkl} I^{hkl} (2\Theta - 2\Theta_0^{hkl}),$$

$$I^{hkl} = I^{hkl}_{instr.} * I^{hkl}_{size} * I^{hkl}_{disl.}$$

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

CMWP - fit:

	<i>u</i>																		
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CMWP - fit – input files format:

1

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2) ind	ex file		3) backgr	ound file	4) instrume	ental profiles file
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CMWP - fit:

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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-K0 and the second contains the intensity values, where K=2*sin(Theta)/lambda and K0 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: Alphal-LaB6

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CMWP - fit - fitting interval:

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If you have instumental profiles, please enter the name of the of the instrumental profile directory: Alpha1-LaB6									
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): 23									
Please specify the value of maxx (in degrees): 120									
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									
Selection of the size function									
Selection of the size function The program will use the spheric size function (default) • The program will use the ellipsoidal size function O The program will disable the size effect O									
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CMWP - fit – settings/initial values:

	Sampling of the simulated powder pattern data	
1	Please specify N1: 1024 Please specify N2: 1024 Please specify the profile cutting parameter (in Two theta degrees): 4	
-	Initial values of the parameters	
1 1 1 1	Please enter the initial value of the parameter "a" (or "a1"): 1 fix: Please enter the initial value of the parameter "a2": 1 fix: Please enter the initial value of the parameter "b": 3 fix: Please enter the initial value of the parameter "c": 1 fix: Please enter the initial value of the parameter "d": 80 fix: Please enter the initial value of the parameter "e": 0.05 fix: Please enter the initial value of the parameter "e": 0.05 fix: Flease enter the initial value of the parameter "e": 0.05 fix: Please enter the initial value of the parameter "e": 0.05 fix: Please enter the initial value of the parameter "e": fix: Please enter the initial value of the parameter "e": 0.05 fix: Please enter the initial value of the parameter "e": fix: Please enter the initial value of the parameter "e": Please enter t	
]	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	

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CMWP	- †1† _	- retiner	nent/t	11 COT	itrol
	LIU				

Peak parameter refinement and weighting

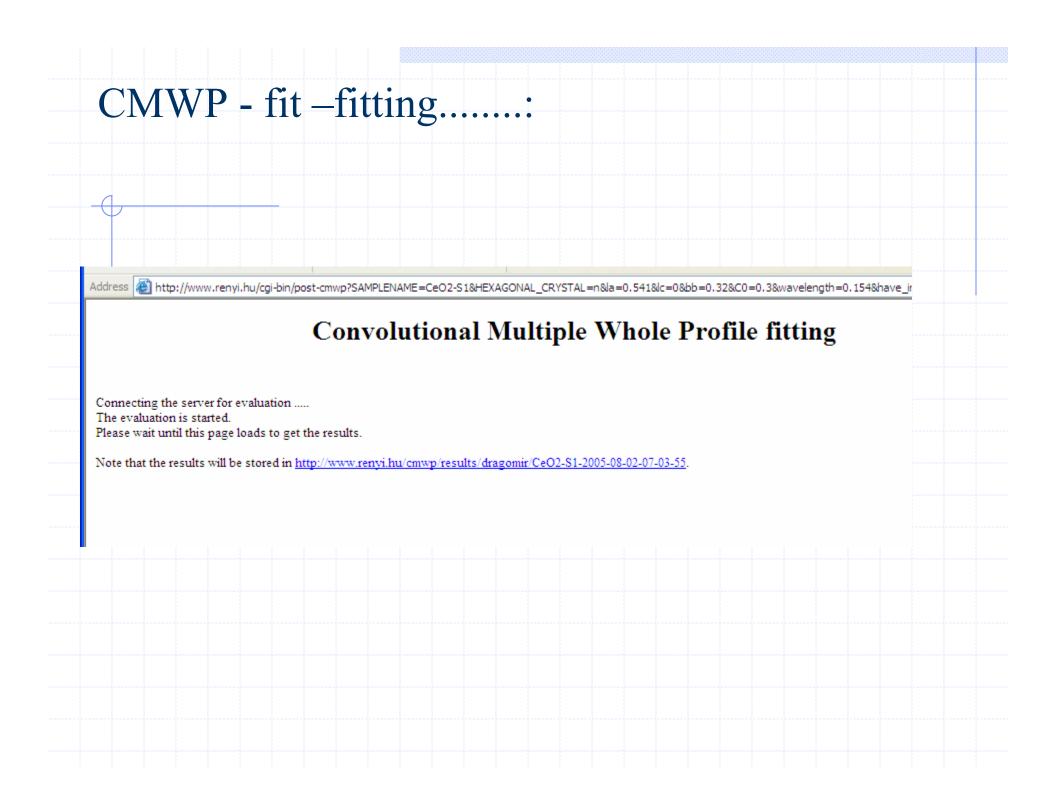
Set this if you want to fit the peak positions and peak intensities:

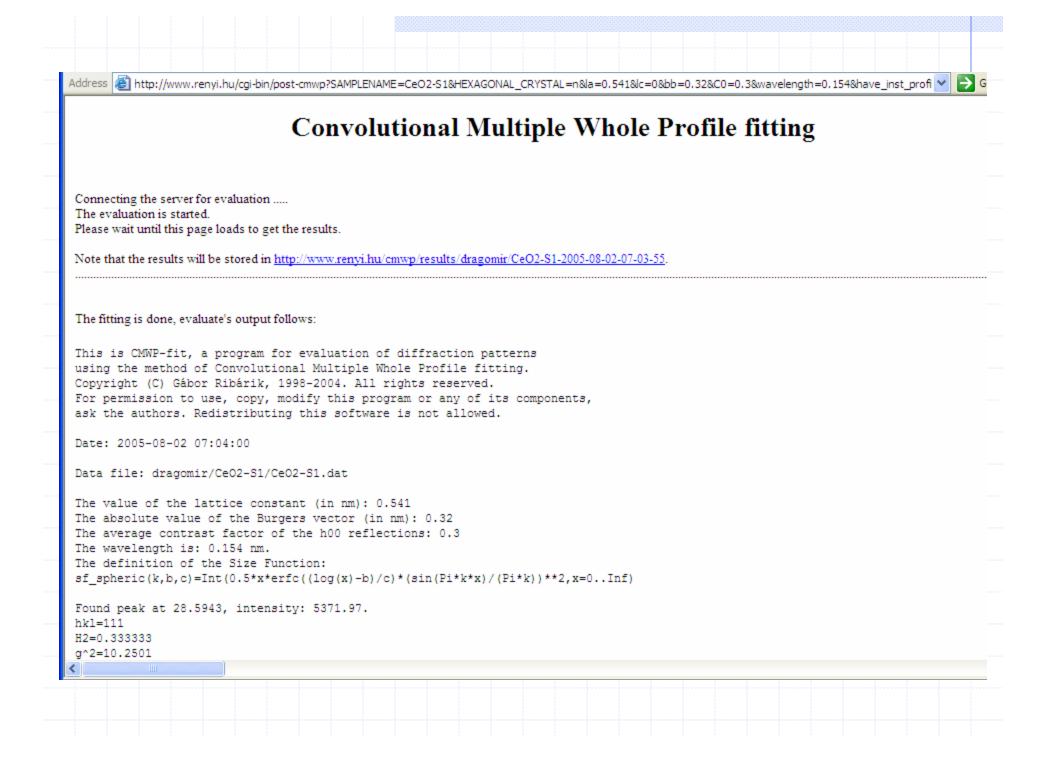
Set this if you want to use weights in the fitting algorithm:

A

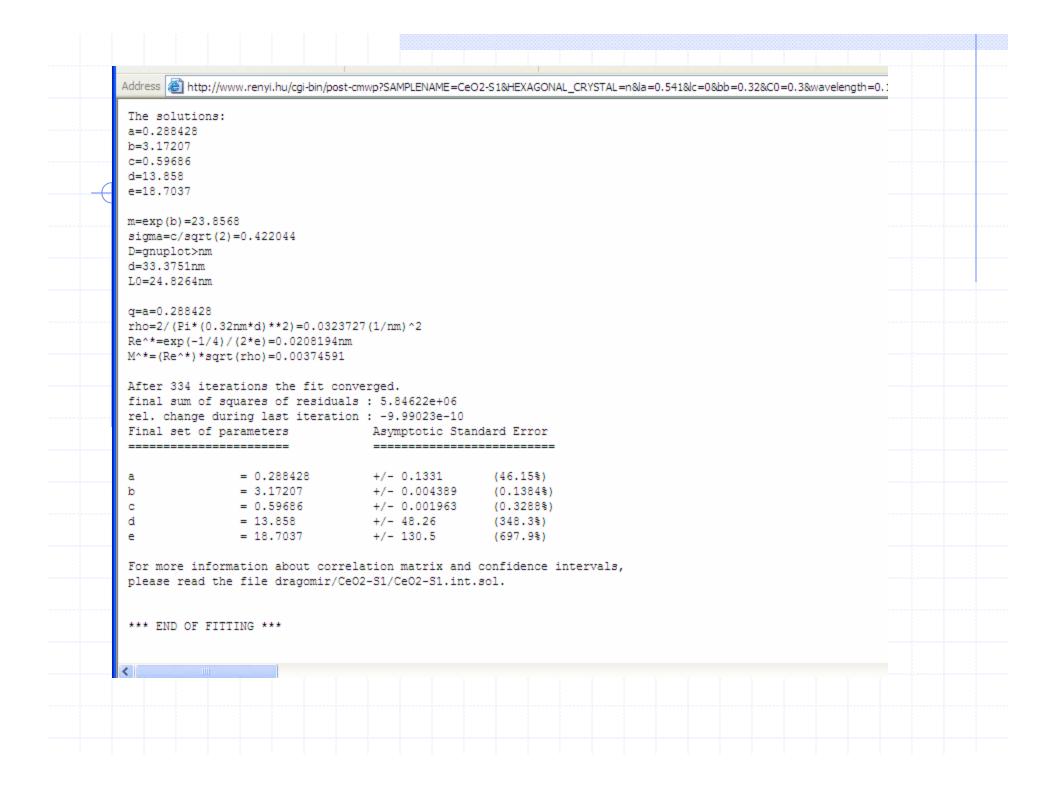
Fit control

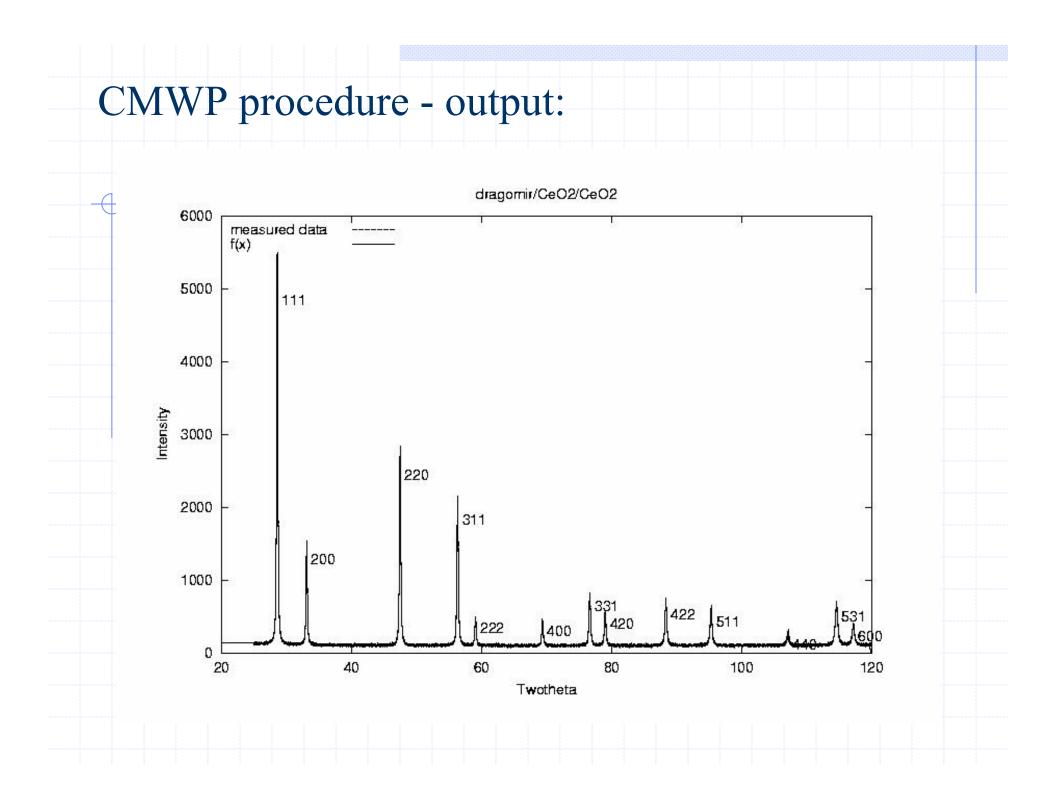
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*** FIT ***							
Calculating a	a,b,c,d,e to fit the	measured powder	diffraction	n pattern			
	responding theoretic						
	values of the parame	eters:					
CO=0.3							
a = 1							
b = 3							
c = 1							
d = 80 e = 0.05							
e = 0.05 epsilon = 1.0	L # FIXED						
	TTAL						
The solutions	3:						
a=0.288428							
b=3.17207							
c=0.59686							
d=13.858							
e=18.7037							
m=exp(b)=23.8	550						
sigma=c/sqrt							
D=gnuplot>nm	(2)-01122011						
d=33.3751nm							
L0=24.8264nm							
q=a=0.288428							
	.32nm*d) **2) =0.03237 4) / (2*e) =0.0208194nm						
	grt(rho)=0.020374591	1					
n ~= (ne ~) ~ 50	10(110)-0.000/4001						
After 334 ite	erations the fit con	werged.					
	squares of residual						
	during last iteratio)				
Final set of	parameters	Asymptotic St	andard Error	r			
a	= 0.288428	+/- 0.1331	(46.15%))			
< 11							





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:			Hexagonal crystal systems:		
<i>m</i> , σ:	\rightarrow	size profile	<i>m</i> , σ	\rightarrow	size profile
	\rightarrow	strain anisotropy	q_1 and q_2	\rightarrow	strain anisotropy
ρ^*, M	\rightarrow	strain profile	ρ^*, M	\rightarrow	strain profile
ρ [,] , ₁ νι	→		$p^{,}$, m	\rightarrow	suam prome

Theoretical individual and average contrast factor of dislocations

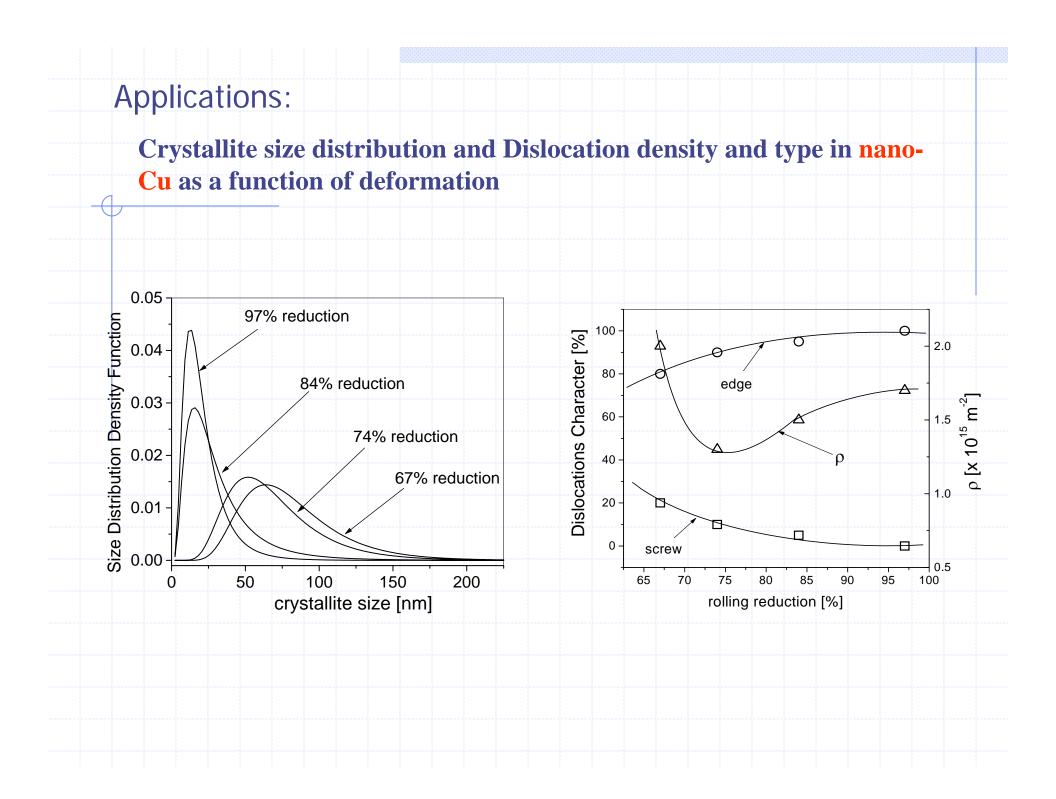
Or can be calculated using ANIZC software at http://metal.elte.hu/anizc/

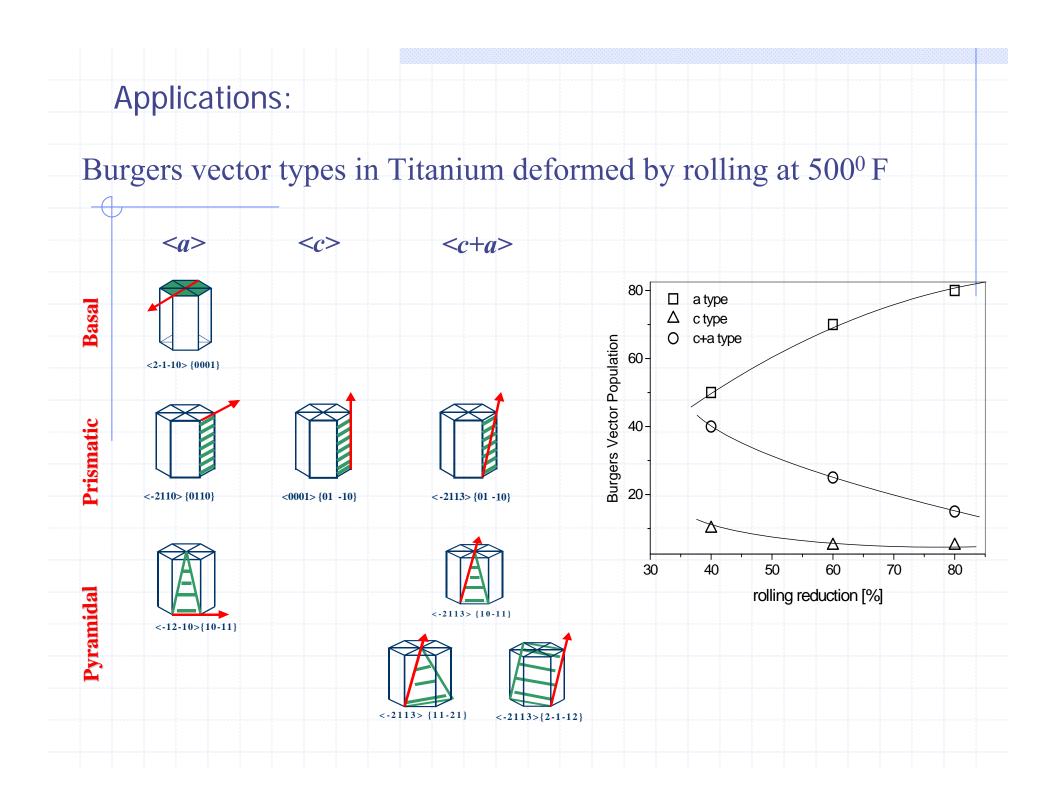
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	ANIZC	C
	Computer program for the calculation of dislocation cubic, hexagonal and trigona	-
	(pleas	ase send any comments or remarks to Andras Borbely at: <u>borbely@ludens.elte.hu)</u>
Please select the crystal system You can find here some <u>Screen</u>		

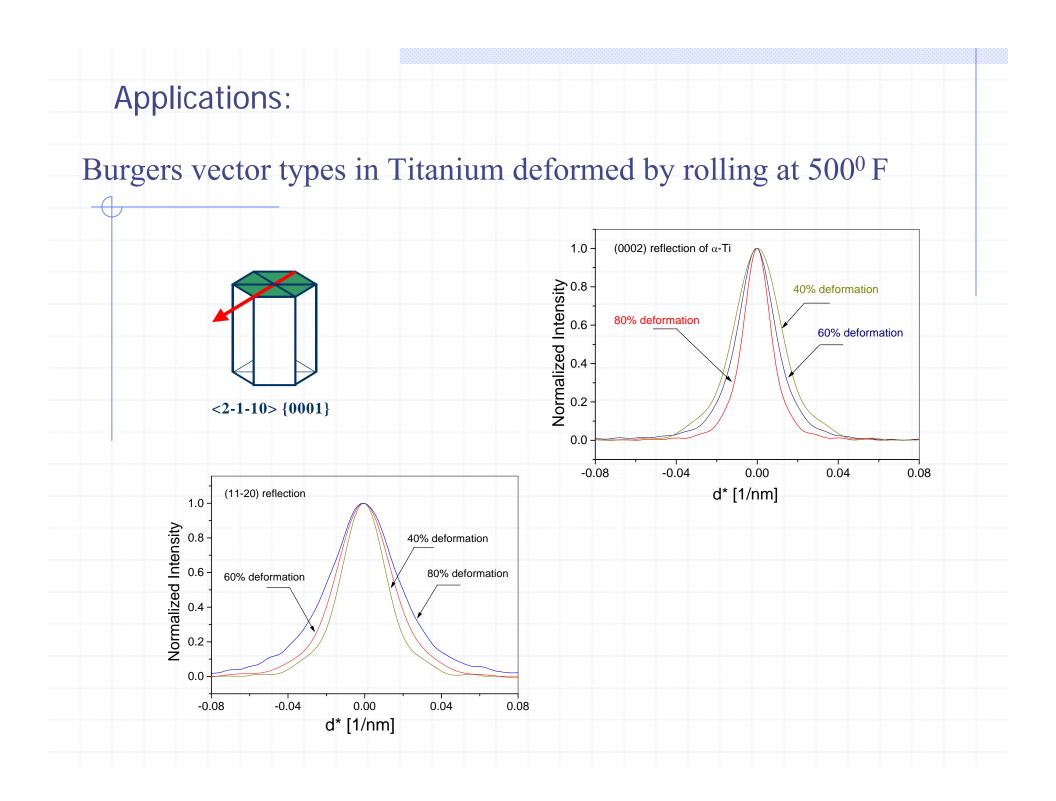
nizC program	was developed by Dr. Ar	ndras Borbely (Department of General
hysics at Eotv	os Science University in H	Budapest, Hungary).
	, , , , , , , , , , , , , , , , , , ,	oárik G. and Ungár T.: "Computer program ANIZC
r the calculation o	f diffraction contrast factors of dis s", in J. Appl. Cryst., 36, 160-162, (islocations in elastically anisotropic cubic, hexagona

Theoretical individual and average contrast factor of dislocations AnizC for cubic crystals Address 🙆 http://metal.elte.hu/anizc/program-cubic.html Google ▼ Yahoo! ▼ Ask Jeeves LookSmart Files ▼ ﷺ Customize 🖑 My Button 🚅 Highlight 📶 Search 👻 **Cubic lattices** Input^{*}: C O or S O c₁₁ c₁₂ C_{44} or or or s₁₂*: s44*: s₁₁*: g* The program computes*: O the individual contrast factor for a single dislocation: b: n: ŀ or the average contrast factor for: ○ edge <110>{111} type dislocations O edge <111>{110} type dislocations O 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 Google ▼ Yahoo! ▼ Ask Jeeves Look Smart Files ▼ 🗱 Customize 🖑 My Button 📶 Search 👻 The Program Anizc $Input^*: C \bigcirc or S \bigcirc$ c₁₁ c₁₂ C_{44} or or or s₄₄*: s₁₁*: s₁₂*: C₁₃ C33 or or s₁₃*: S33*: c/a*: g*: The program computes*: O the individual contrast factor for a single dislocation: b: n: ŀ or the average contrast factor for: edge <-12-10>{10-10} type dislocations O edge <-12-10>{10-11} type dislocations edge <-2110>{0001} type dislocations O edge <-2113>{01-10} type dislocations 🙆 Done







Summary

MWP or CMWP procedure enables the determination of the sample microstructure form 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.*

<u>Ribarik Gabor</u> for continuous help provided in the preparation

of the present tutorial.