



X-ray Diffraction

- Basic aspects of x-ray crystallography and powder diffraction
- Diffraction from nanocrystalline materials

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Special thanks to: Luca Gelisio, Alberto Leonardi, Luca Rebuffi, Cristy L. Azanza Ricardo, Mirco D'Incau, Andrea Troian, Emmanuel Garnier, Mahmoud Abdellatief



PRESENTATION OUTLINE

PART I

Diffraction from nanocrystalline materials:
why using synchrotron radiation?

PART II

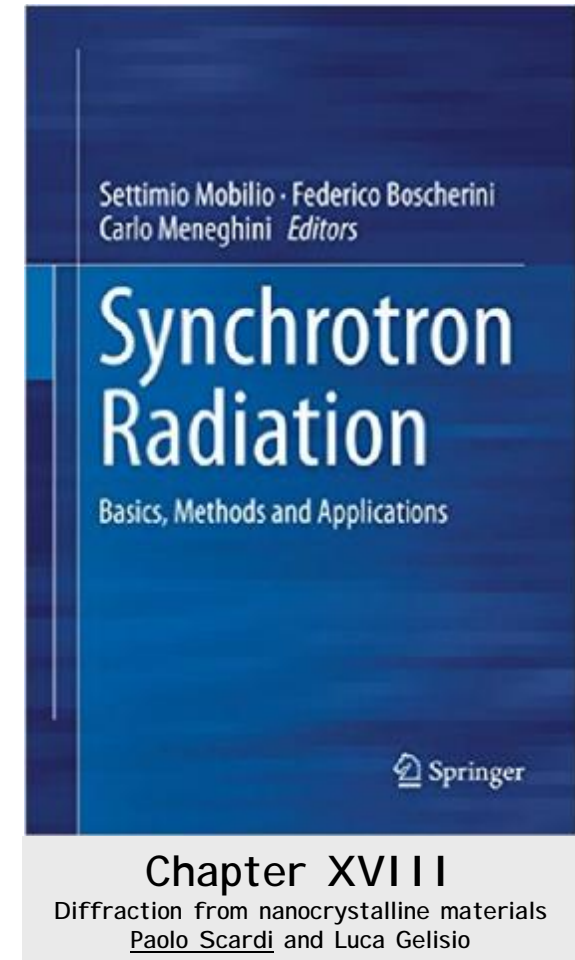
Reciprocal space vs direct
space methods

PART III

Selected case studies:
highly deformed metals,
and nanocrystalline catalyst

PART IV

Total Scattering methods





SYNCHROTRON RADIATION X-RAY DIFFRACTION

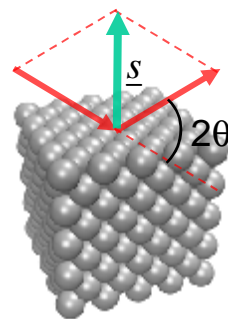
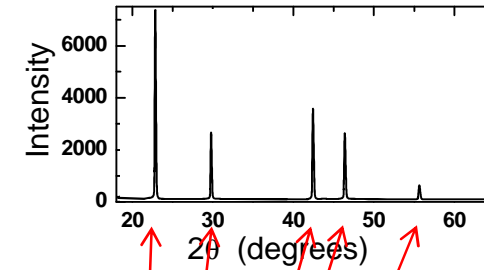
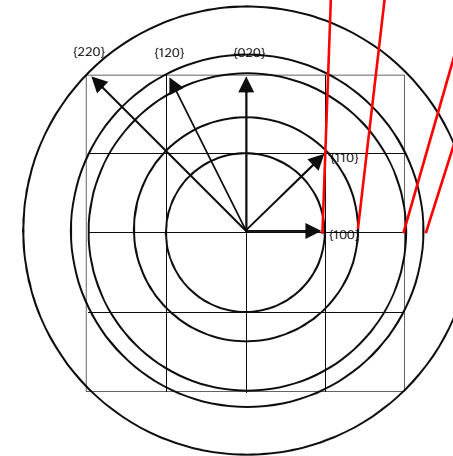
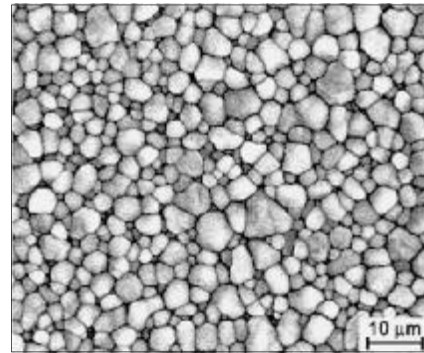
main applications of (powder / polycrystalline material) diffraction

- Crystal structure determination: structure solution and refinement.
- Line Profile Analysis (LPA): crystalline domain size/shape, lattice defect analysis – nanocrystalline materials
- Phase Identification (Search-Match procedures): pure crystalline phases or mixtures
- Quantitative Phase Analysis (QPA): crystalline and amorphous phases
- Texture Analysis (TA): determination of preferred orientations
- X-ray Residual Stress Analysis (XRSA): measurement of strain field / elastic behaviour

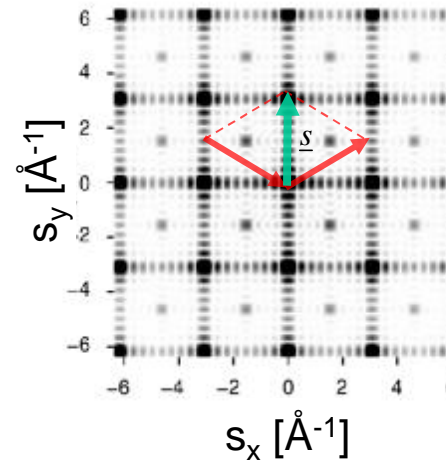


DIFFRACTION PATTERN FROM A POLYCRYSTALLINE

powder
(bulk polycrystalline)



$$s = Q/2\pi = 2\sin\theta / \lambda$$





SYNCHROTRON RADIATION X-RAY DIFFRACTION

from single-crystal to powder diffraction

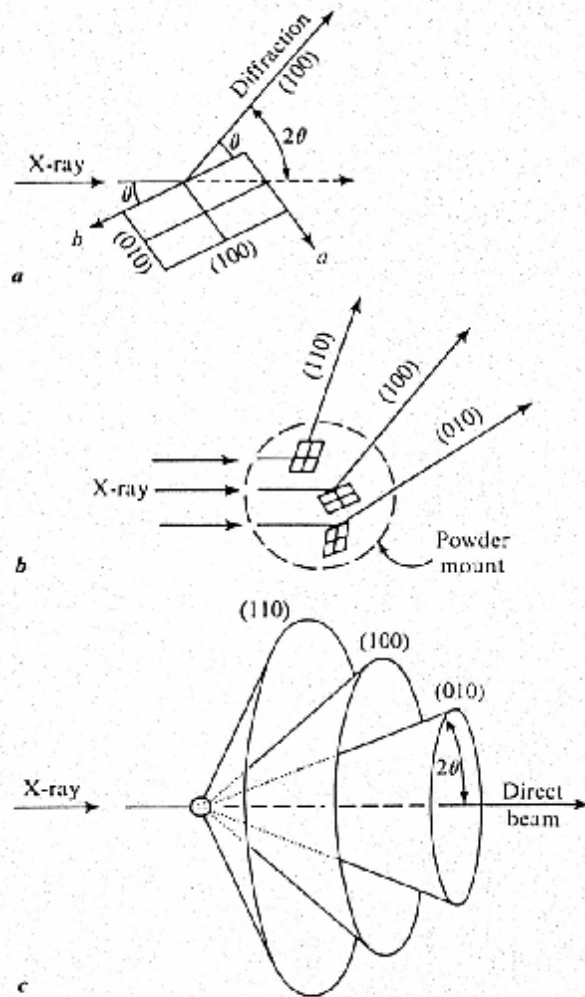
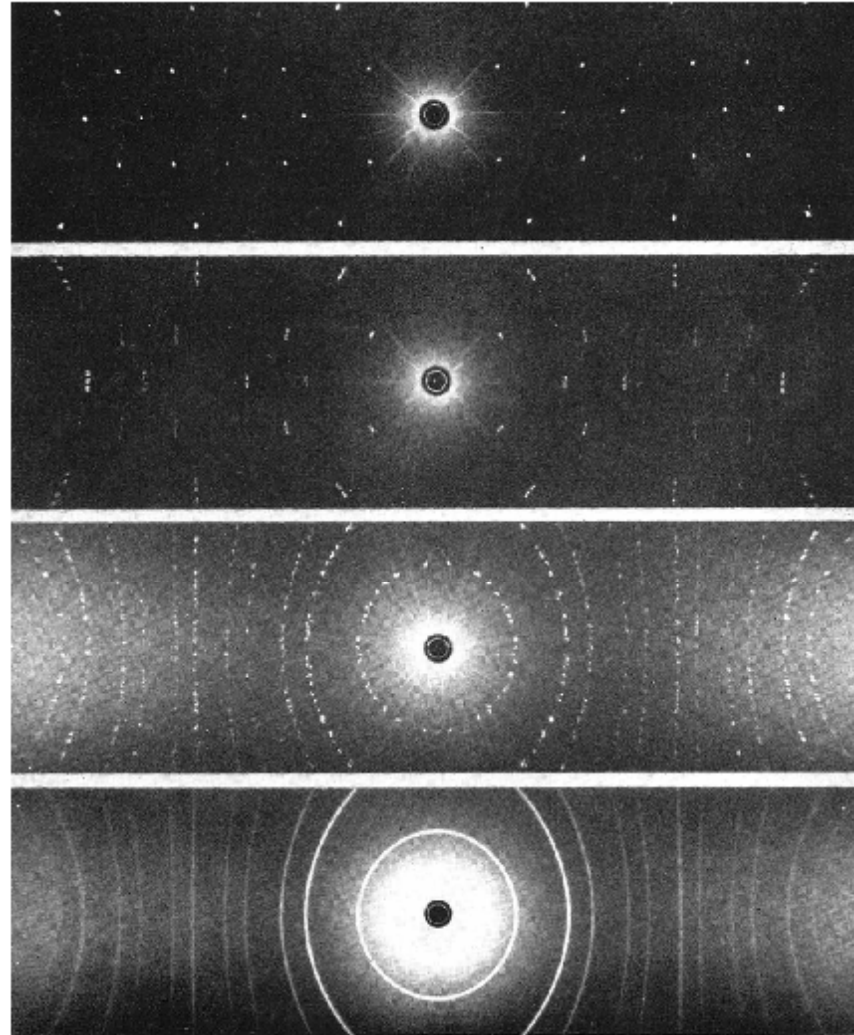


FIGURE 10.11 Diffraction of monochromatic x-rays from (a) a single crystal and (b) an aggregate of small mineral fragments. (c) Diffraction cones produced by the powder method.

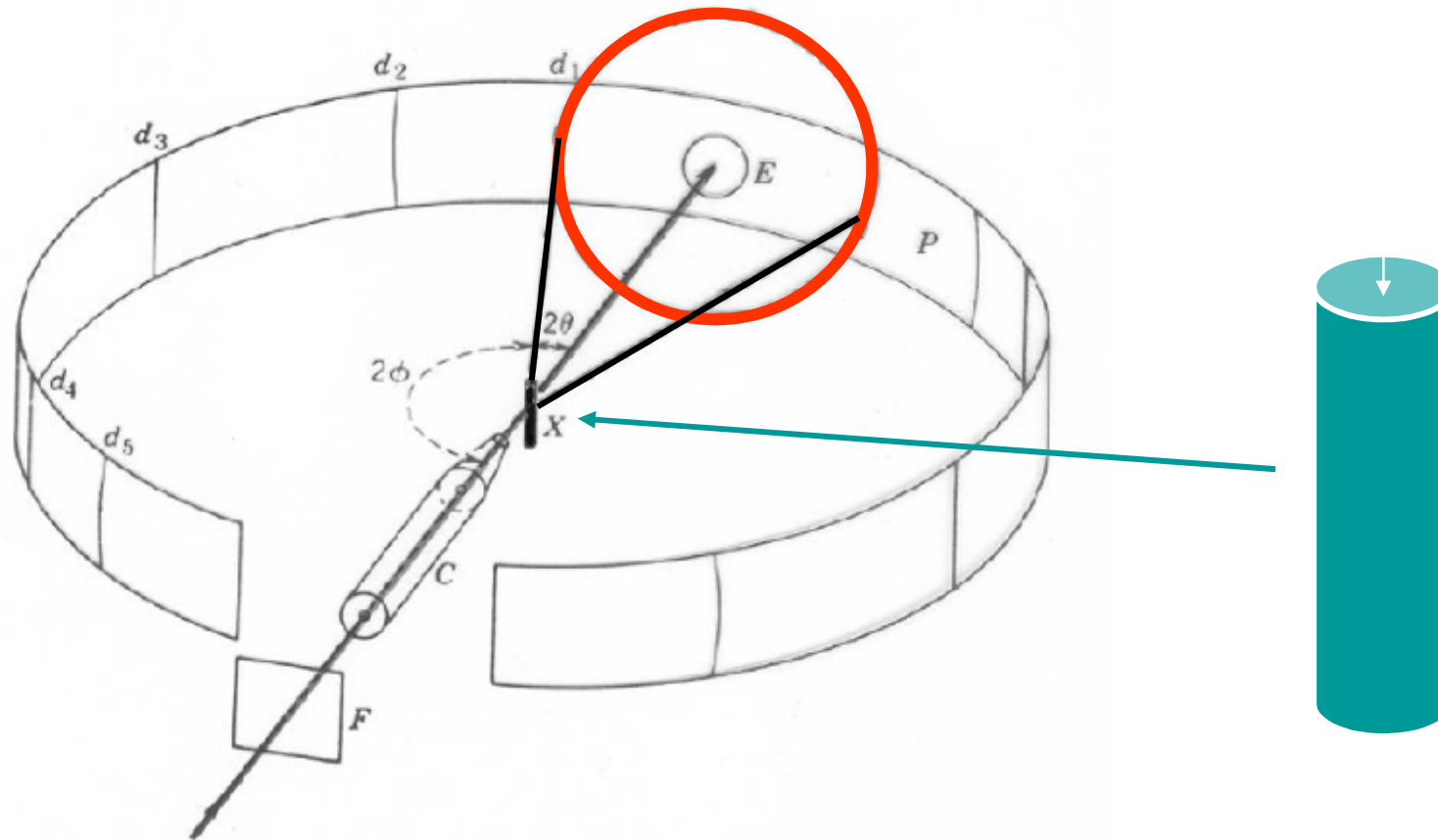


(From top to bottom). Fig. 197; Single-crystal rotation photograph of fluorite [100] vertical; Fig. 198; Single-crystal rotation photograph of fluorite [100] 2° to vertical; Fig. 199; X-ray photograph of five randomly oriented crystals of fluorite; Fig. 200; Powder photograph of fluorite.



SYNCHROTRON RADIATION X-RAY DIFFRACTION

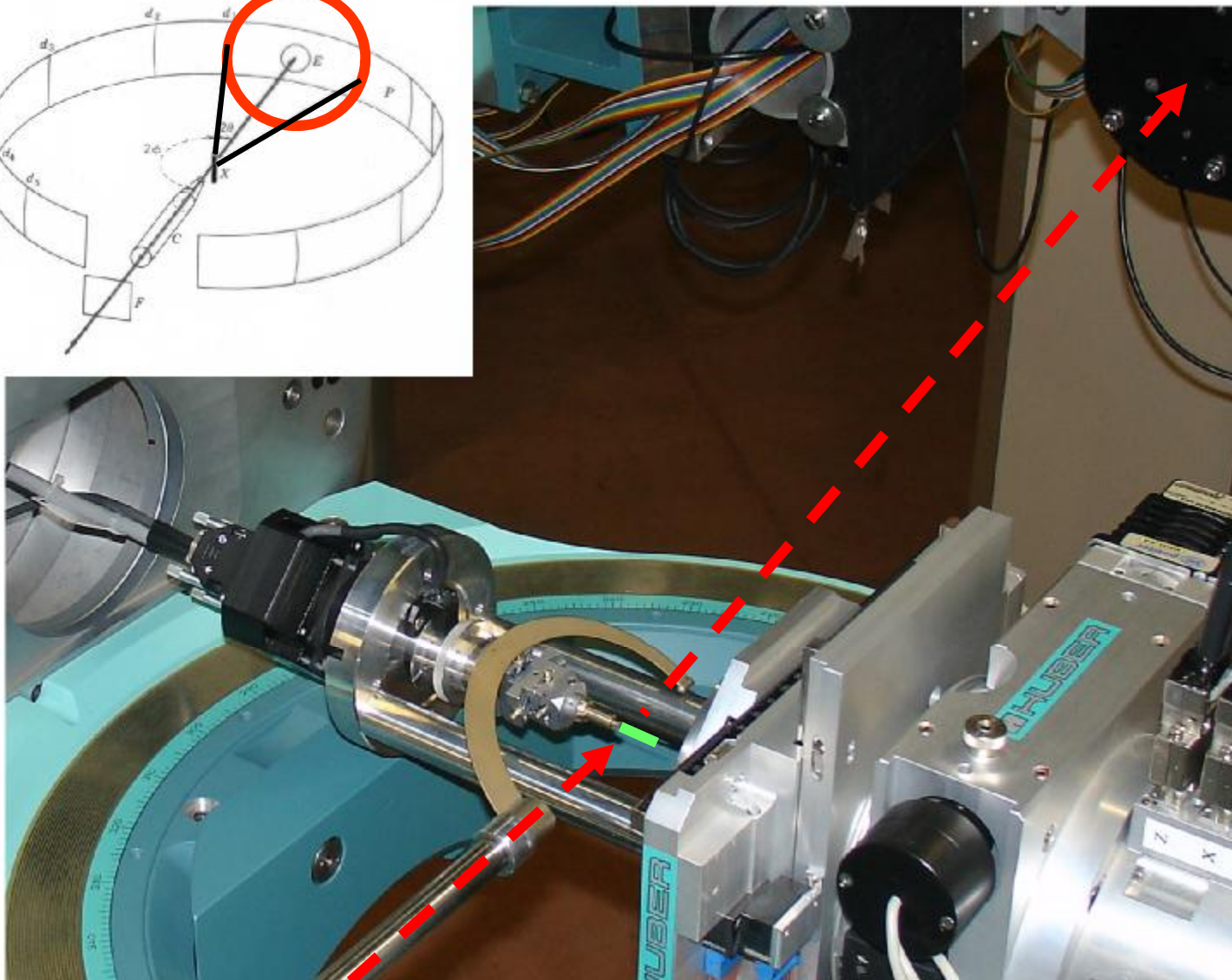
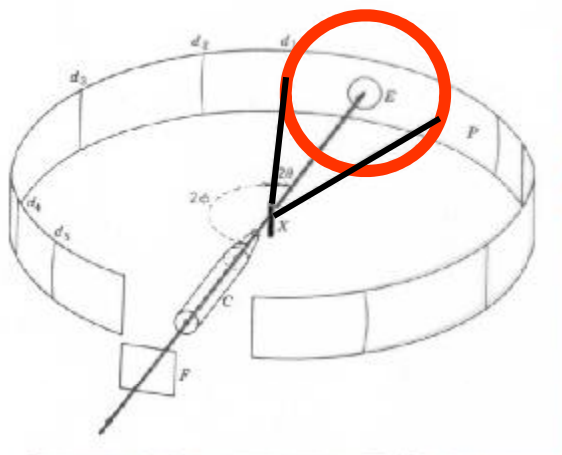
Powder diffraction 'elective' geometry: Debye-Scherrer (1918)





SYNCHROTRON RADIATION X-RAY DIFFRACTION

parallel beam, Debye Sherrer geometry of MCX (ELETTRA)

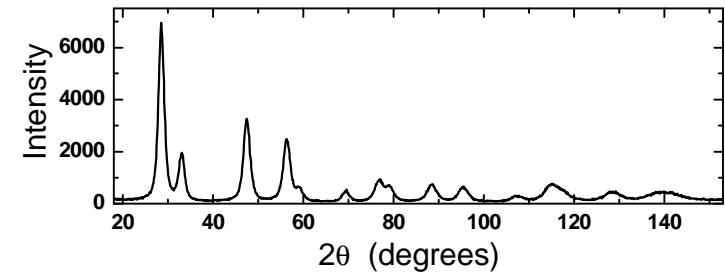
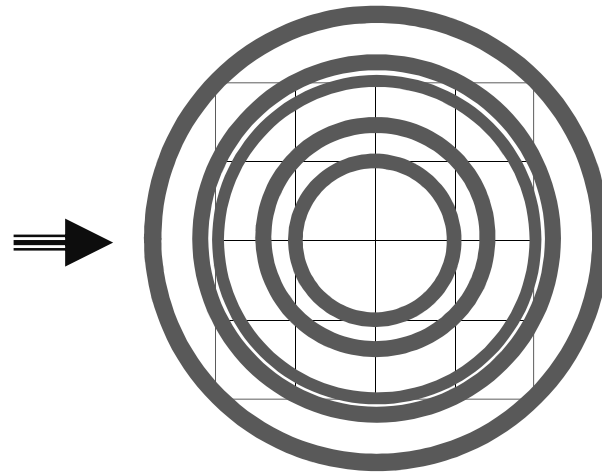
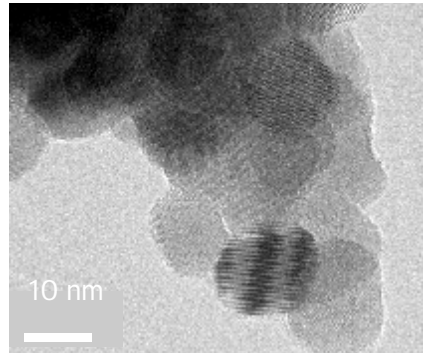




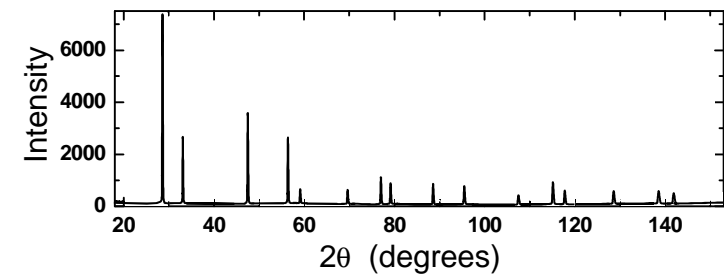
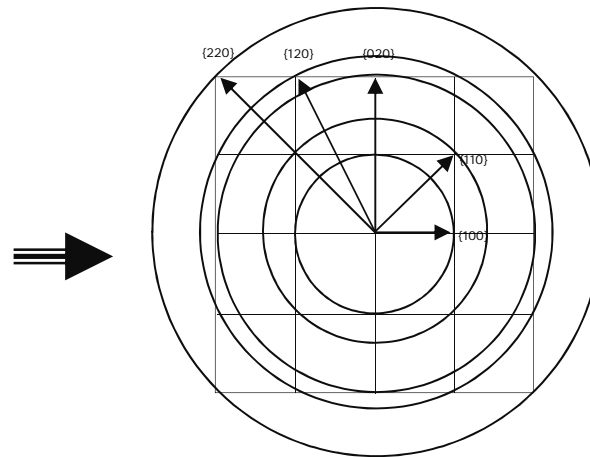
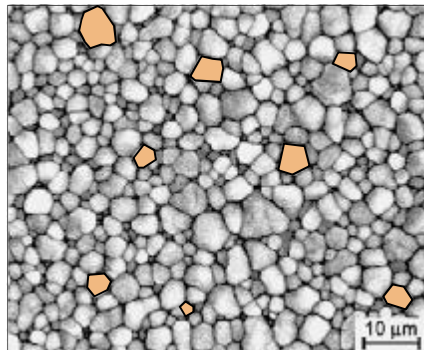
DIFFRACTION PATTERN FROM A POLYCRYSTALLINE

peaks from nanocrystals are broad: why using SR ???

nanocrystalline powder



powder (bulk polycrystalline)

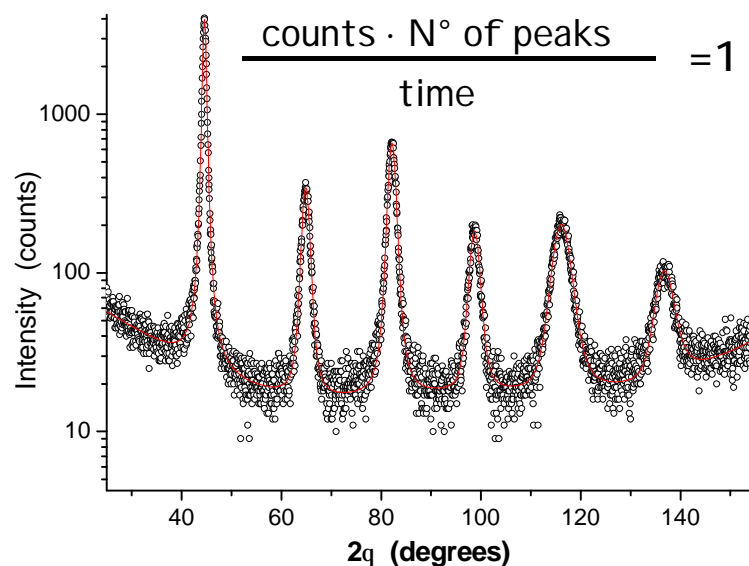




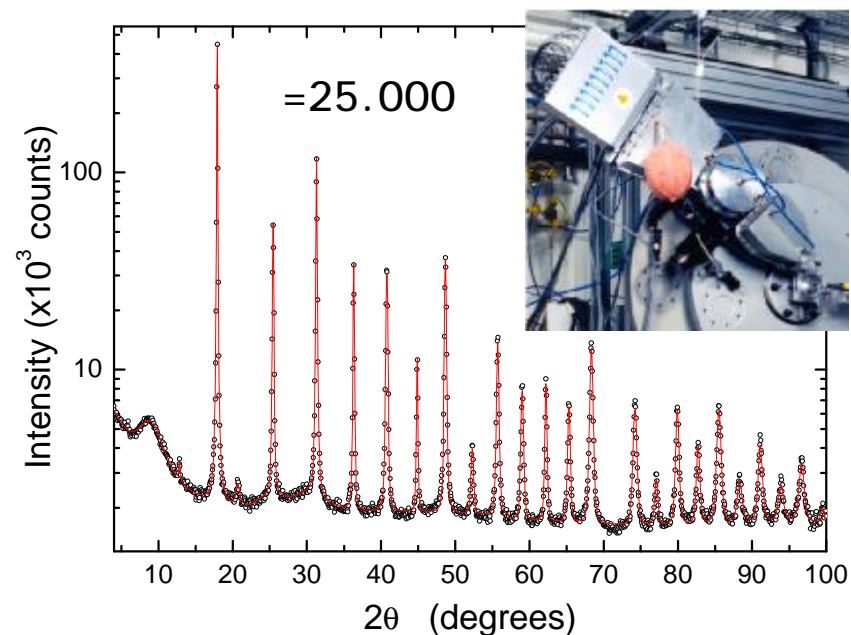
SYNCHROTRON RADIATION X-RAY DIFFRACTION

- high brilliance: better counting statistics / shorter data collection time / fast kinetics, in situ, in operando studies

Lab instrument: ~80.000s



9-crystal analyzer: 1.500s ! (x100 counts)



CuK α $\lambda=0.15406$ nm

ESRF ID31 (now ID22) $\lambda=0.0632$ nm

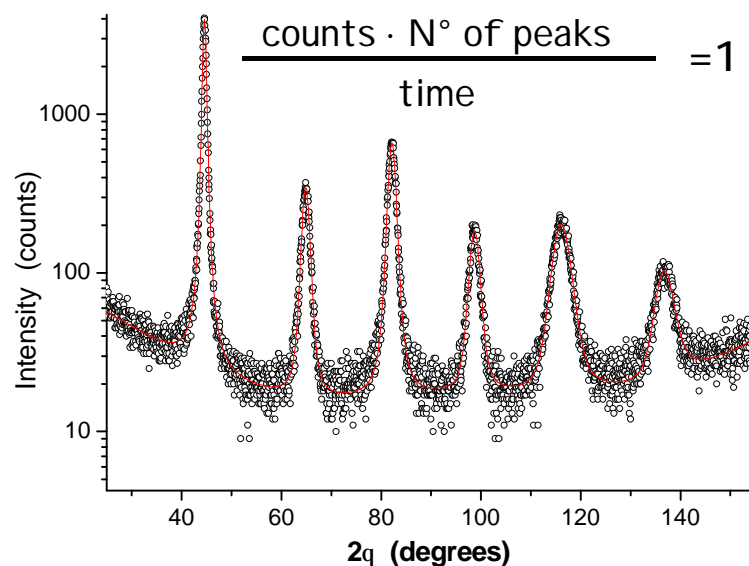
iron powder (ball milled)



SYNCHROTRON RADIATION X-RAY DIFFRACTION

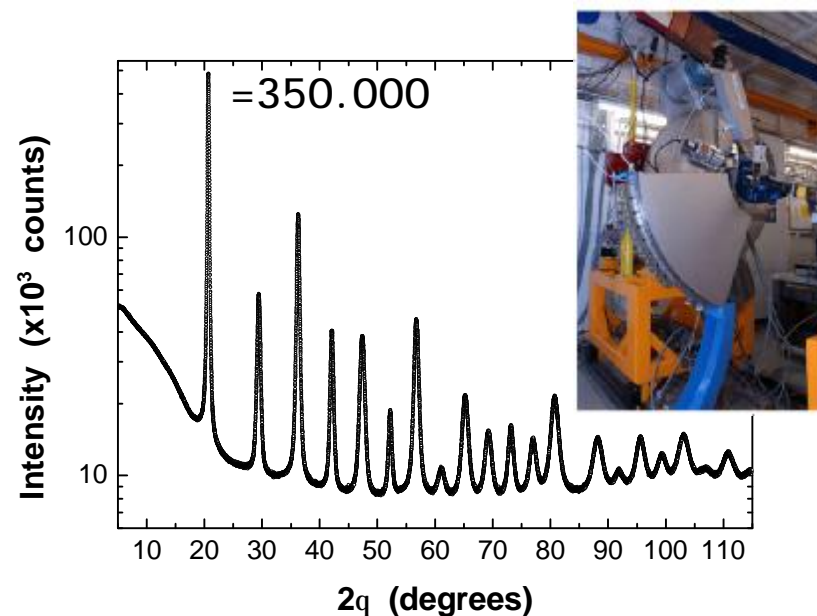
- high brilliance: better counting statistics / shorter data collection time / fast kinetics, in situ, in operando studies

Lab instrument: ~80.000s



CuK α $\lambda=0.15406$ nm

Mythen detector: 100 s !! (x100 counts)



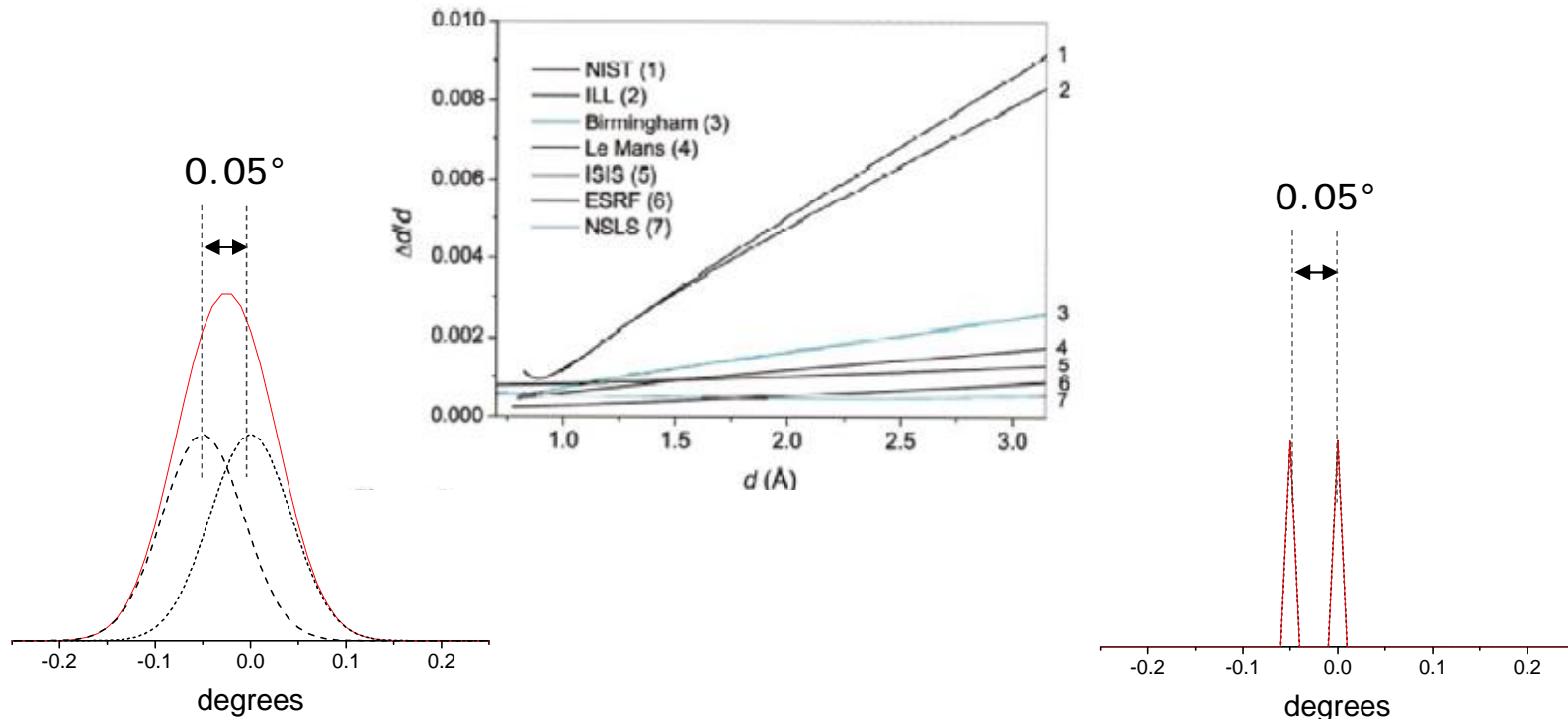
PSI MS-X04SA $\lambda=0.072929$ nm

iron powder (ball milled)



SYNCHROTRON RADIATION X-RAY DIFFRACTION

- narrow instrumental profile: control of instrumental profile; high resolution and accuracy in measuring peak position, intensity and profile width/shape



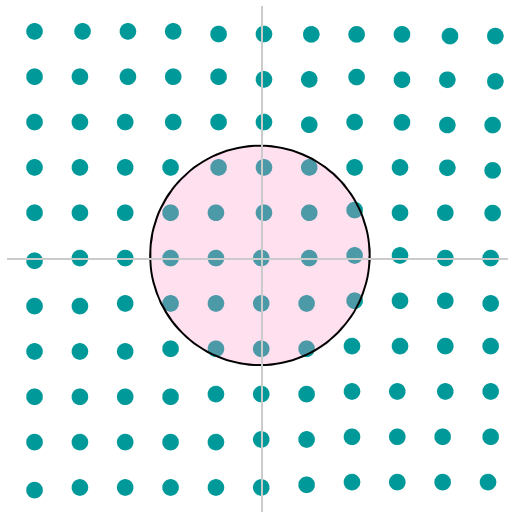
Lab instrument:
FWHM ≈ 0.05 - 0.1°

ID31 @ESRF:
FWHM ≈ 0.003 - 0.004°

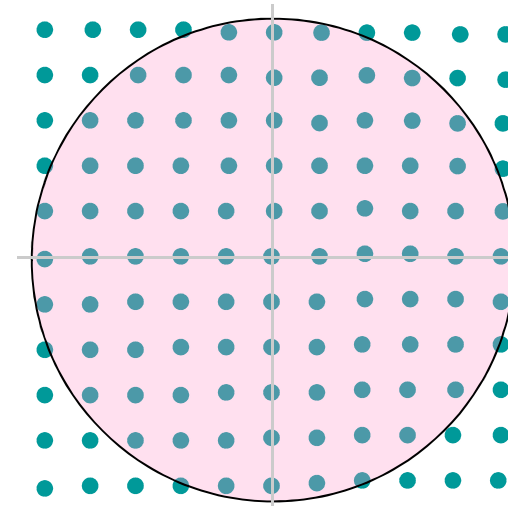


SYNCHROTRON RADIATION X-RAY DIFFRACTION

- extending the accessible region of reciprocal space well beyond what traditional lab instruments can make



λ_1



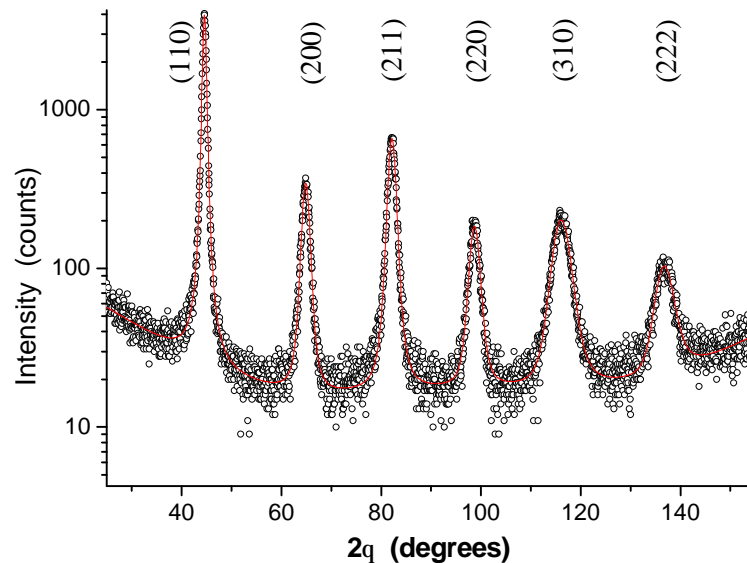
$\lambda_2 < \lambda_1$



SYNCHROTRON RADIATION X-RAY DIFFRACTION

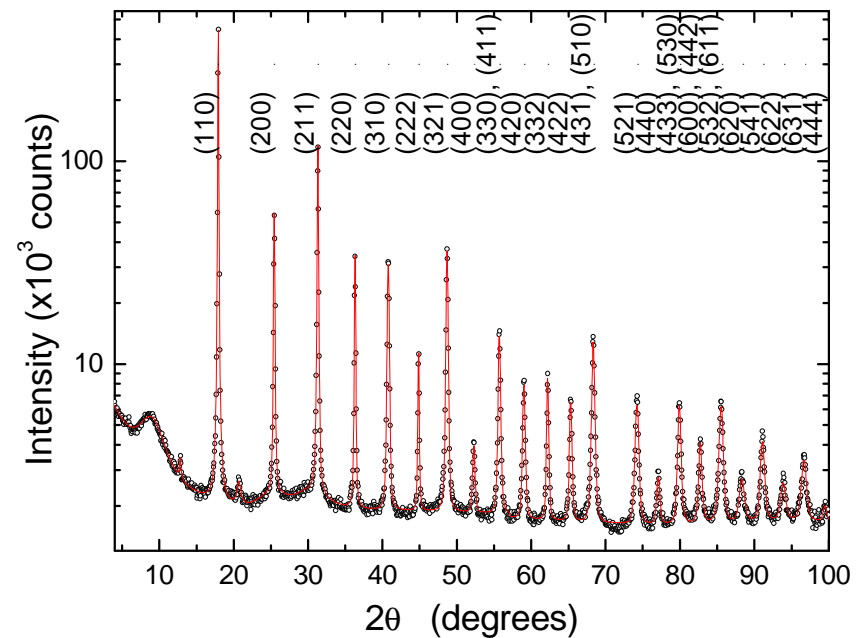
- extending the accessible region of reciprocal space well beyond what traditional lab instruments can make

Lab instrument: ~80.000s
: 6 peaks



CuK α $\lambda=0.15406$ nm

9-crystal analyzer: 1.500s ! (x100 counts)
: 28 peaks

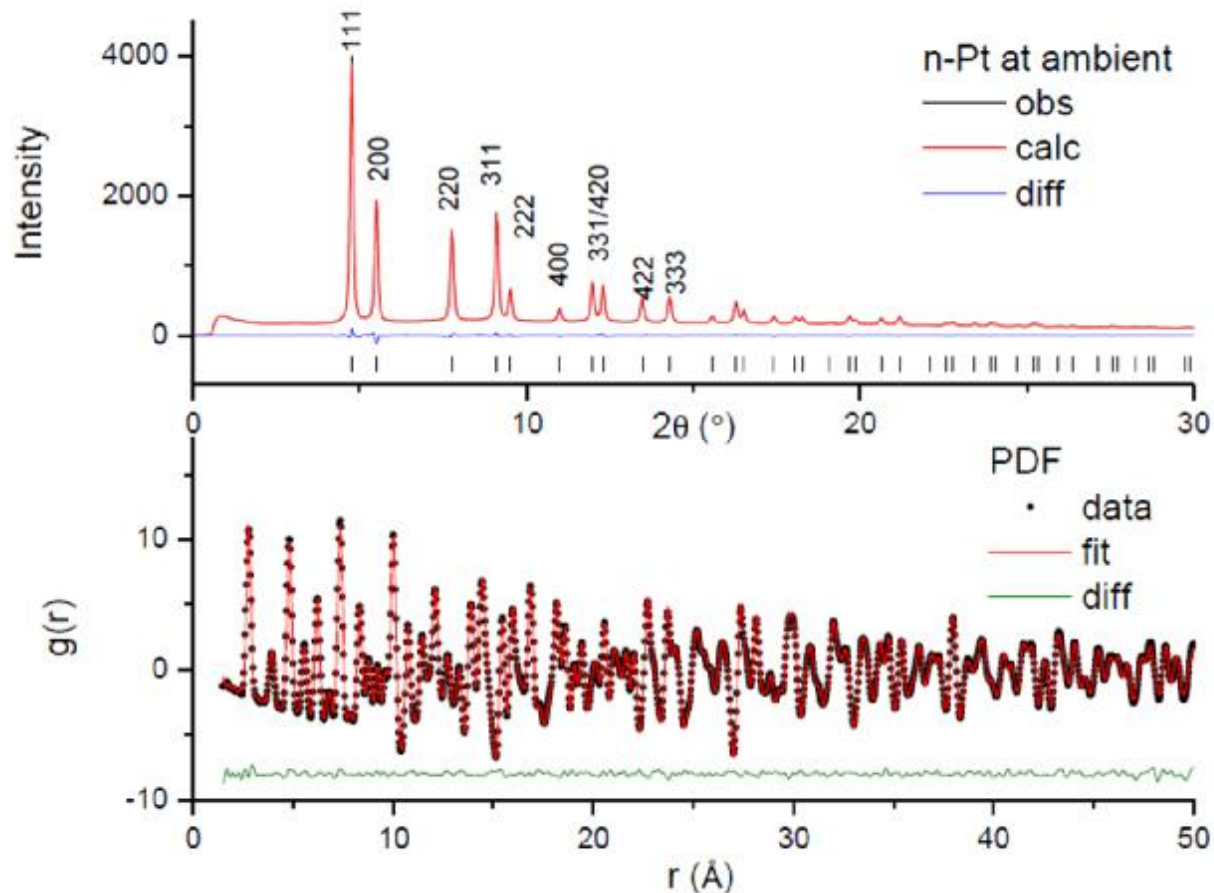


ESRF ID31 $\lambda=0.0632$ nm



SYNCHROTRON RADIATION X-RAY DIFFRACTION

- extending the accessible region of reciprocal space well beyond what traditional lab instruments can make: PDF analysis

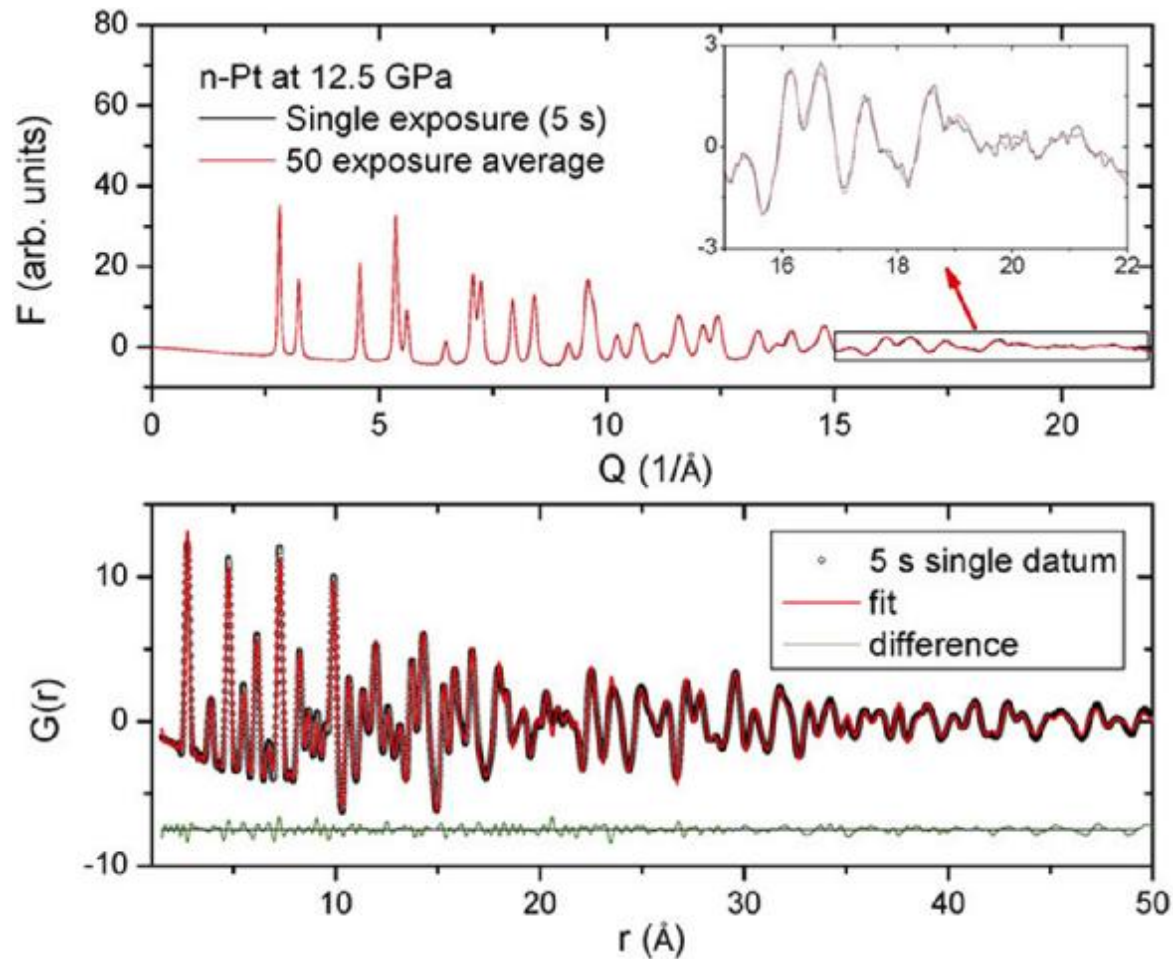


High-pressure pair distribution function (PDF) measurement of nano Pt (50 nm) at 12.5 GPa in Methanol:Ethanol = 4:1. Focused X-ray beam, 66.054 keV, Brookhaven National Laboratory. Hong et al., Nat. Sci. Reports 6, 21434 (2016)



SYNCHROTRON RADIATION X-RAY DIFFRACTION

- extending the accessible region of reciprocal space well beyond what traditional lab instruments can make: PDF analysis

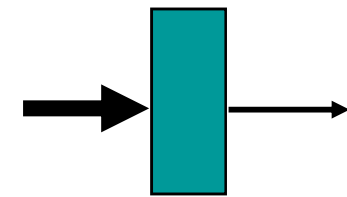
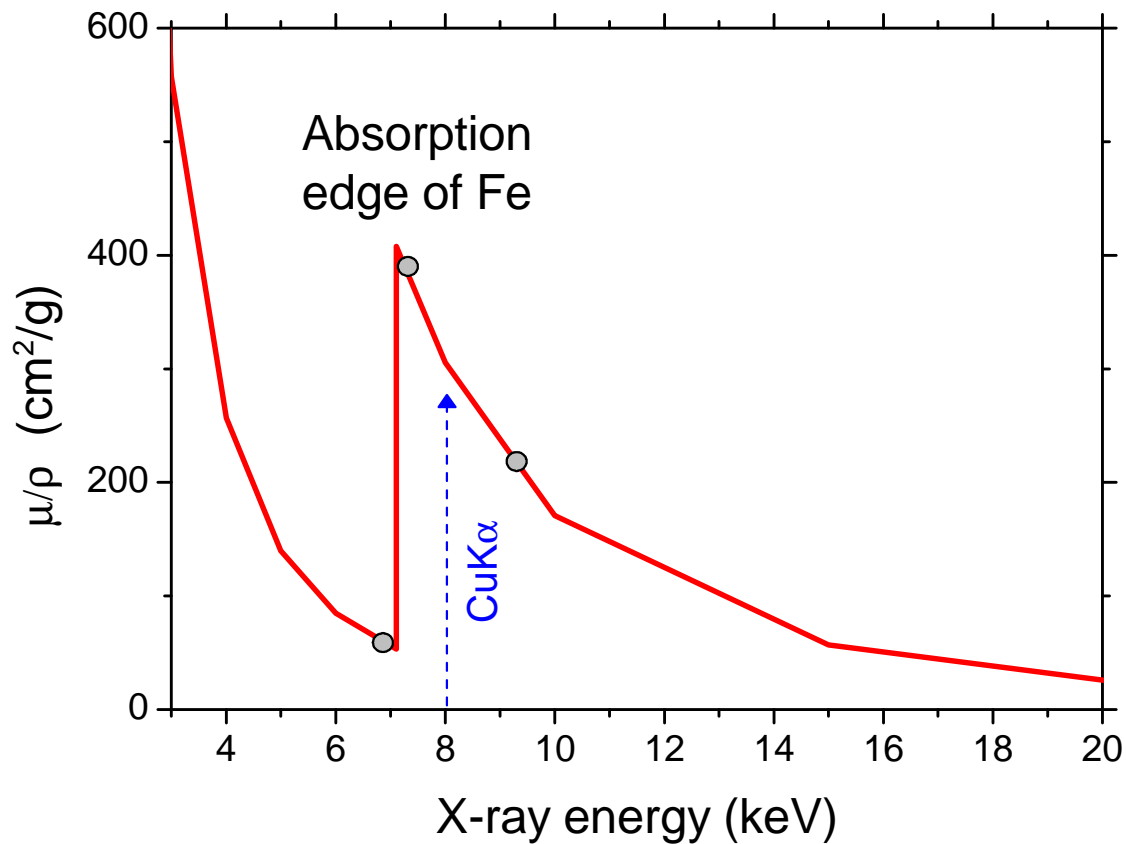


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SYNCHROTRON RADIATION X-RAY DIFFRACTION

- tuning energy according to adsorption edges for, e.g.: resonant scattering, in depth measurements (property gradients)



$$I = I_0 e^{-\left(\frac{\mu}{\rho}\right) \rho t}$$

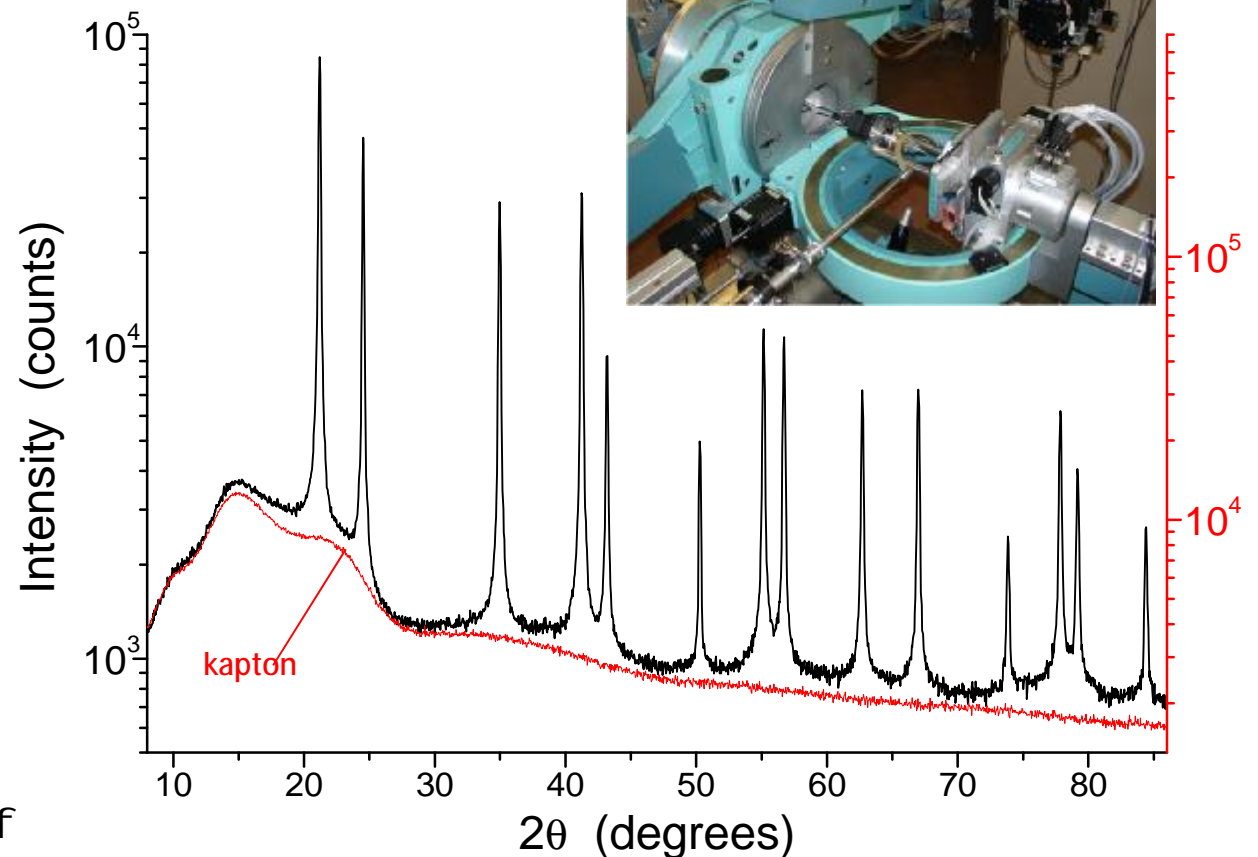


SYNCHROTRON RADIATION X-RAY DIFFRACTION

- tuning energy according to adsorption edges for, e.g.:
resonant scattering, in depth measurements (property gradients);
control fluorescence emission and *absorption*

MCX beamline (Elettra), 15 keV

Negligible absorption: $\mu=2.71 \text{ cm}^{-1}$ $\Rightarrow \mu R \approx 0.07$

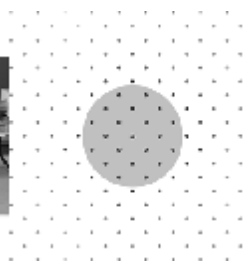
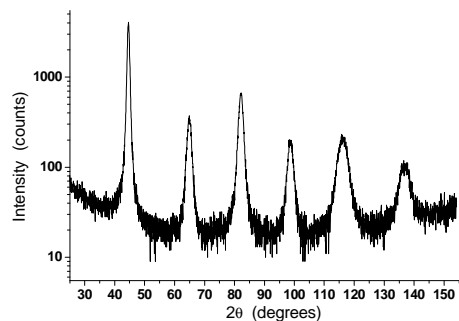


Special thanks to: M. Abdellatief



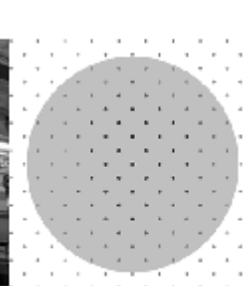
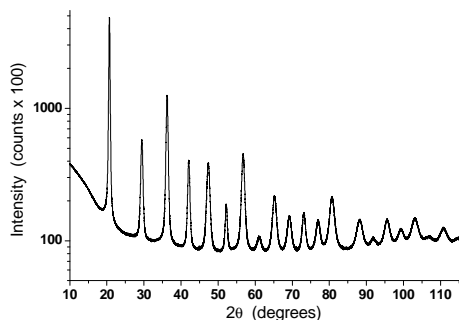
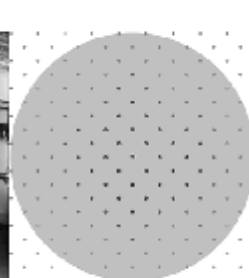
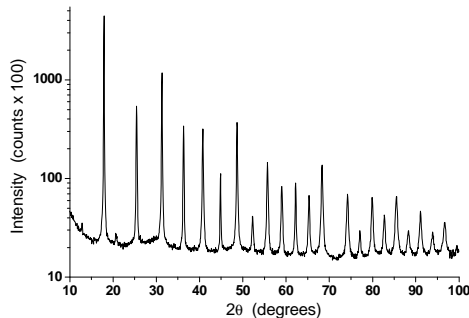
SYNCHROTRON RADIATION X-RAY DIFFRACTION

- increase energy \Rightarrow extend Ewald sphere!
- increase energy \Rightarrow high $Q(=4\pi\sin\theta/\lambda)$ for PDF analysis
- statistics /short time /kinetics / in situ / in operando
- control absorption and instrumental effects



Powder diffraction data from a ball milled Fe1.5%Mo powder collected (a) on a traditional laboratory instrument (Rigaku PMG-VH, Bragg-Brentano geometry) with CuK α radiation ($\lambda=0.1540598$ nm) and SR (Debye-Scherrer geometry): (b) ID31 (now ID22) at ESRF, Grenoble (F) ($\lambda=0.0632$ nm), and (c) MS-X04SA at PSI, Villigen (CH) ($\lambda=0.072929$ nm). On the right: schematic of reciprocal space with extension of the limiting sphere (radius $2/\lambda$).

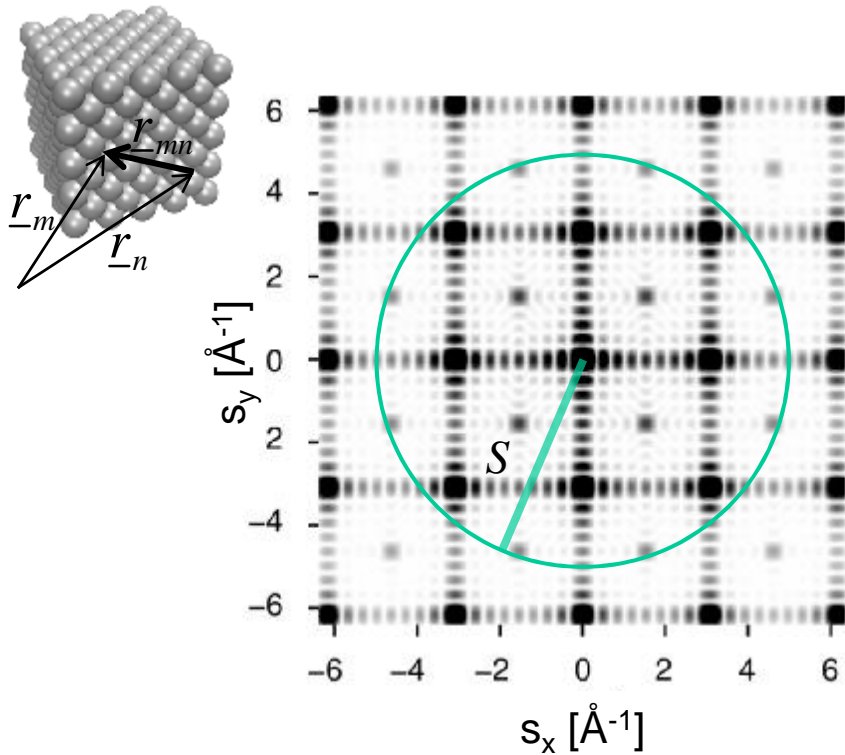
P. Scardi & L. Gelisio, "Diffraction from nanocrystalline materials", in Synchrotron radiation, ed. S. Mobilio et al., Springer 2015. Chap. XVIII.



**Powder diffraction and synchrotron radiation:
visit the MCX beamline at ELETTRA ([J.R. Plaisier](#))**



DIFFRACTION FROM NANOCRYSTALLINE POWDER



$$s = Q/2\pi = 2\sin\theta / \lambda$$

orientational
(or powder)
average



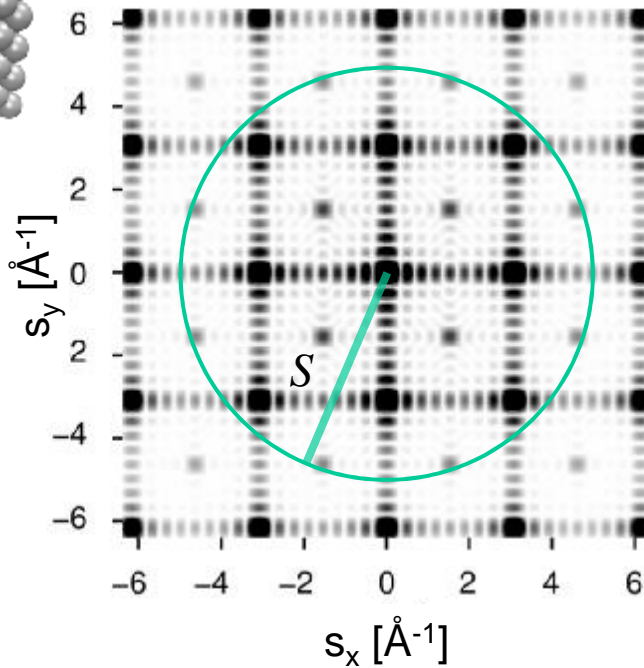
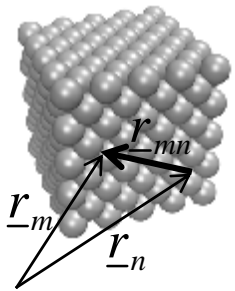
$$I_{PD}(s) \propto \frac{\int I_{sc}(\underline{s}) d\Omega}{4\pi s^2}$$

$$d\Omega = s^2 \sin J dJ df$$

$$I_{sc}(\underline{s}) \propto \sum_m f_m e^{2\pi i(\underline{s} \cdot \underline{r}_m)} \sum_n f_n^* e^{-2\pi i(\underline{s} \cdot \underline{r}_n)} = \sum_m \sum_n f_m f_n^* e^{2\pi i(\underline{s} \cdot \underline{r}_{mn})}$$



DIFFRACTION FROM NANOCRYSTALLINE POWDER



Traditional "reciprocal space" approach
 (1) sum, then average
 or
 (2) average, then sum
 Debye scattering equation, "direct space"
 Total scattering approach

$$I_{PD}(s) \propto \frac{\int \sum_m \sum_n f_m f_n^* e^{2\pi i(\underline{s} \cdot \underline{r}_{mn})} d\Omega}{4\pi s^2}$$

$$\underline{s} = Q/2\pi = 2\sin\theta / \lambda$$

$$d\Omega = s^2 \sin J dJ df$$

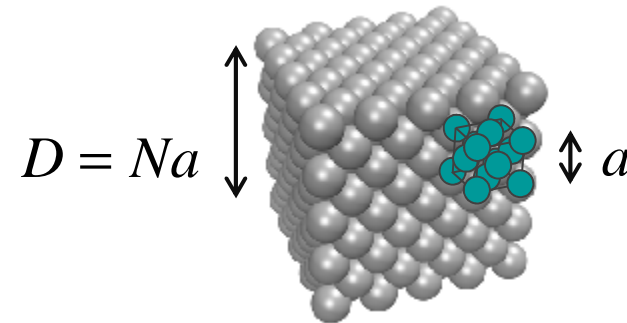
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DIFFRACTION FROM NANOCRYSTALLINE POWDER

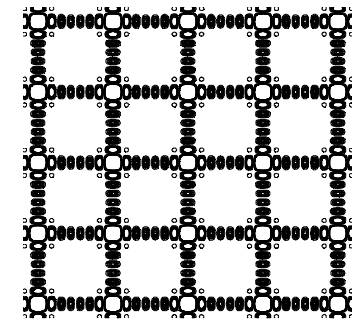
Traditional "reciprocal space" approach (sum, then average)

1. Factorize the contribution of a unit cell
($|F|^2 = F$, structure factor)



2. Build the diffraction signal as interference between unit cells

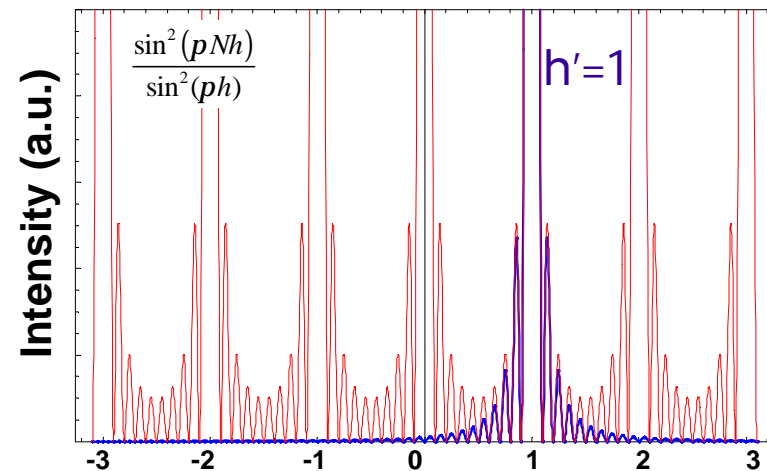
$$I_{sc} \propto |F|^2 \sum_{h'=-\infty}^{\infty} \sum_{k'=-\infty}^{\infty} \sum_{l'=-\infty}^{\infty} \frac{\sin^2(pNh)}{p^2(h-h')^2} \frac{\sin^2(pNk)}{p^2(k-k')^2} \frac{\sin^2(pNl)}{p^2(l-l')^2}$$



Integral Breadth (b) of a ($h00$) peak:

$$b = \frac{\int_{-\infty}^{\infty} \frac{\sin^2(pNh)}{p^2(h-1)^2} dh}{I(h=1)} = \frac{N}{N^2} = \frac{1}{N} \propto \frac{1}{D}$$

Scherrer equation

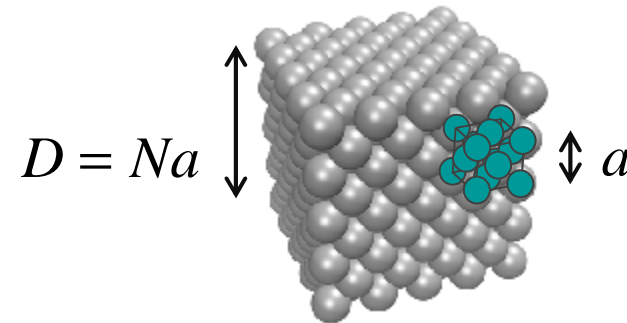




DIFFRACTION FROM NANOCRYSTALLINE POWDER

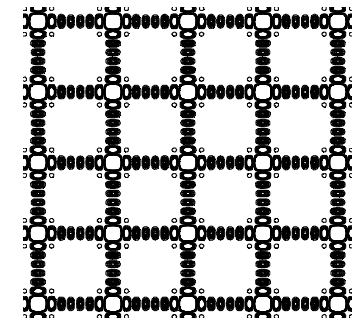
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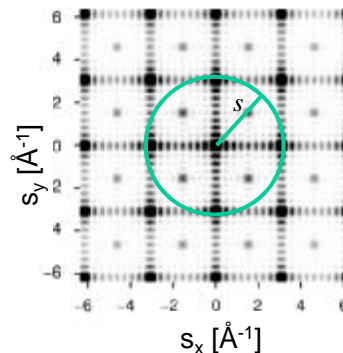
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- Integrate over the powder diffraction sphere (orientational average)

$$I_{PD}(s) \propto \frac{\int I_{sc}(\underline{s}) d\Omega}{4\pi s^2}$$



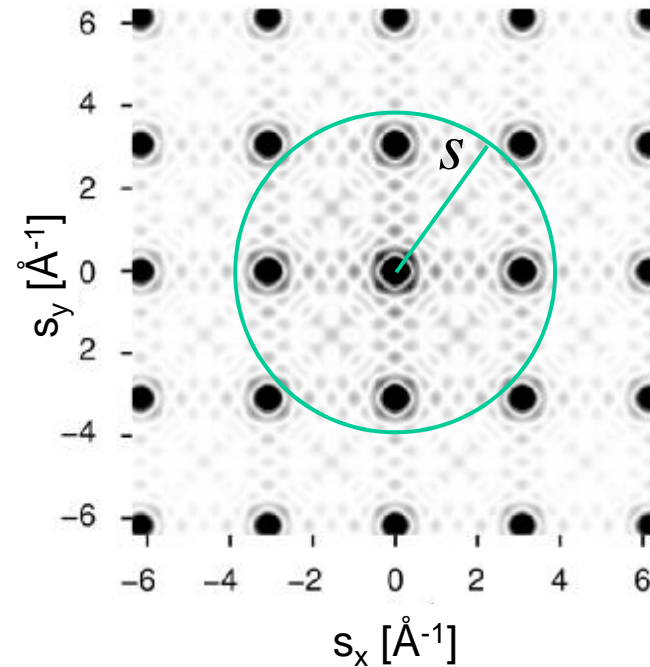
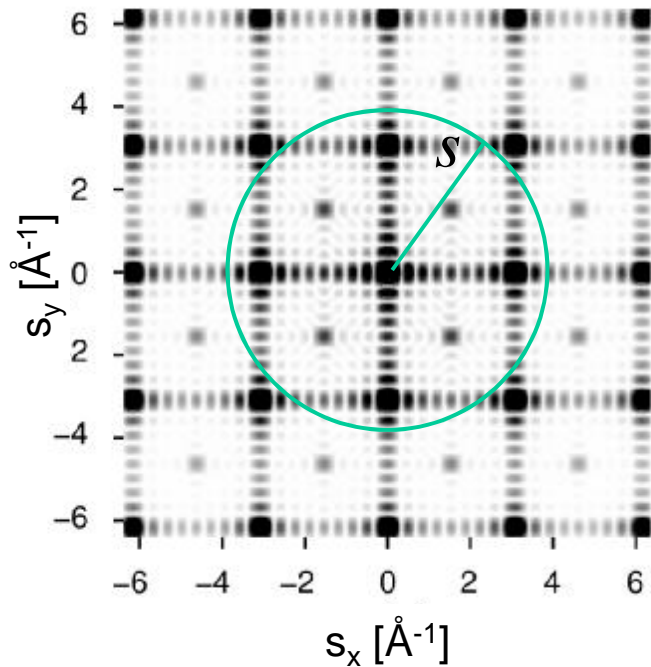
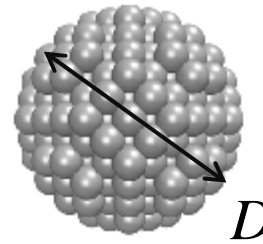
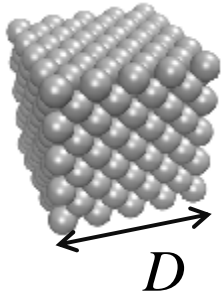
$$I(q) \propto |F|^2 \Phi(q, D)$$

line profile function



DIFFRACTION FROM NANOCRYSTALLINE POWDER

small cubic / spherical fcc domains



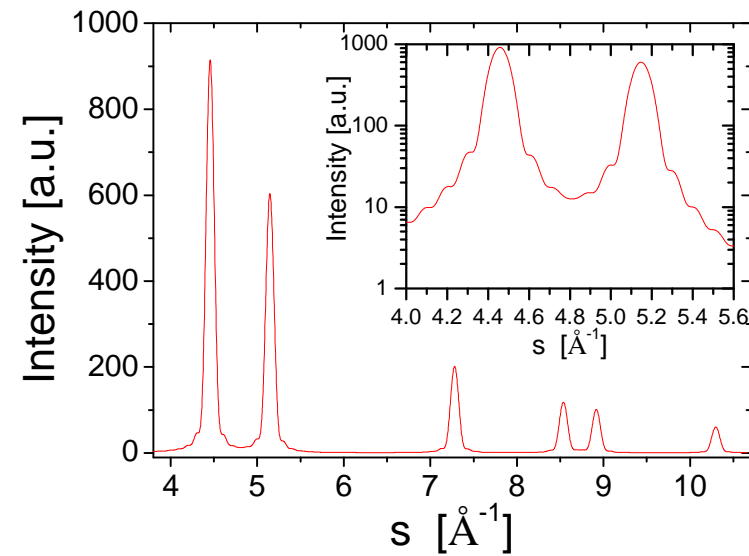
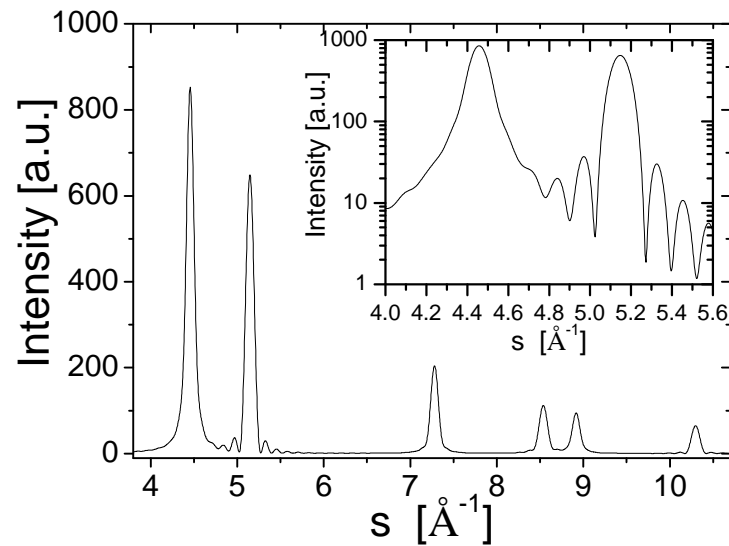
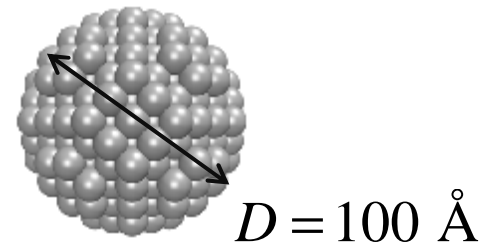
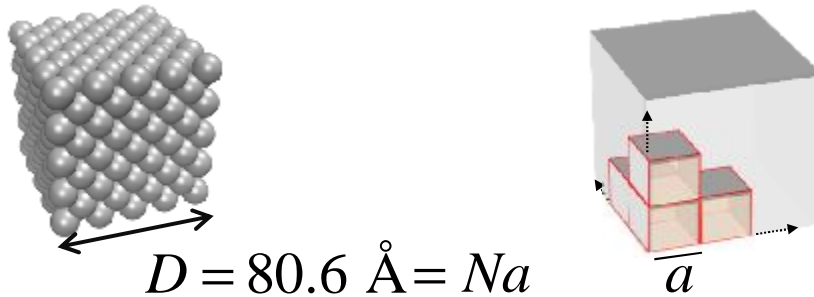
$$I_{PD}(s) \propto |F|^2 \Phi_{cube}(s, D)$$

$$I_{PD}(s) \propto |F|^2 \Phi_{sphere}(s, D)$$



DIFFRACTION FROM NANOCRYSTALLINE POWDER

small cubic / spherical fcc domains



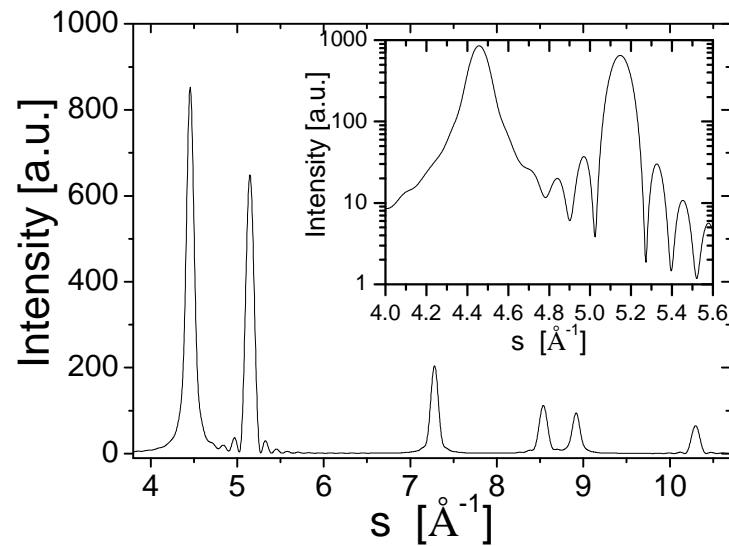
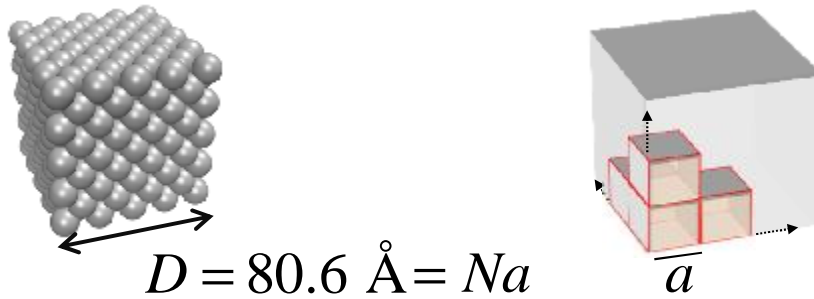
$$I_{PD}(s) \propto |F|^2 \Phi_{cube}(s, D)$$

$$I_{PD}(s) \propto |F|^2 \Phi_{sphere}(s, D)$$



IDEAL vs REAL NANOCRYSTALS

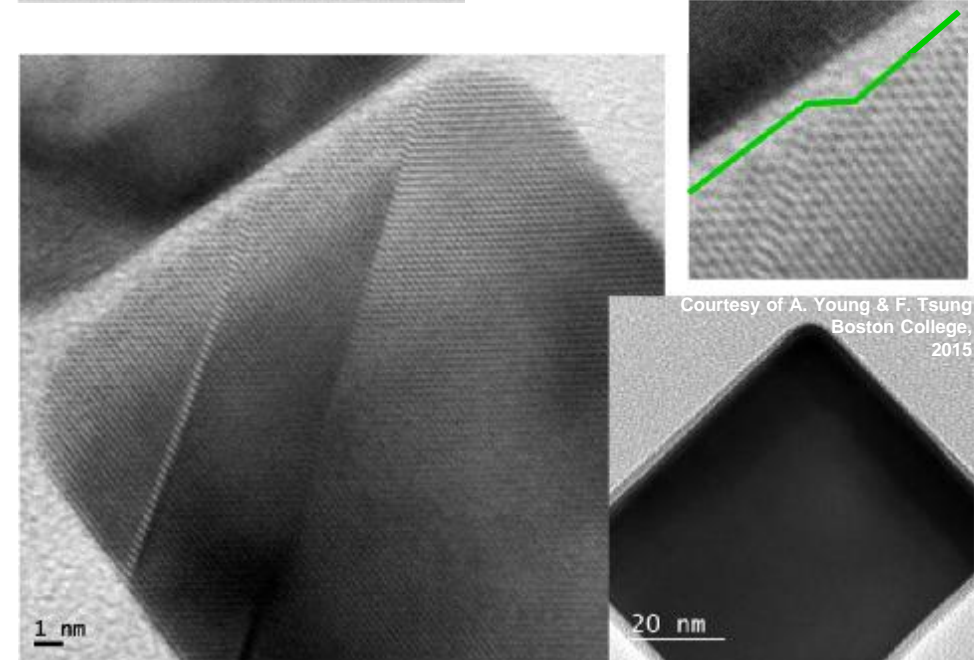
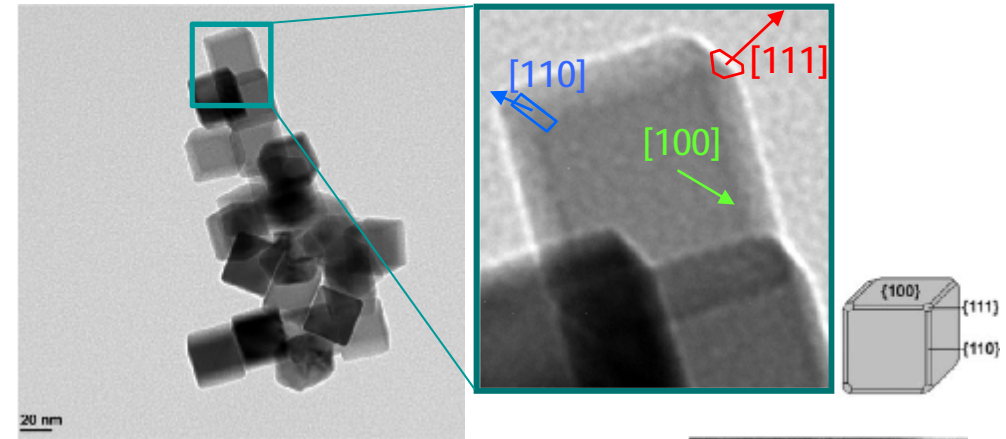
Microstructure: any deviation from perfect crystalline order



$$I_{PD}(s) \propto |F|^2 \Phi_{cube}(s, D)$$

Pd nanocrystals

Solla-Gullon et al., J. Appl. Cryst. 48 (2015) 1534

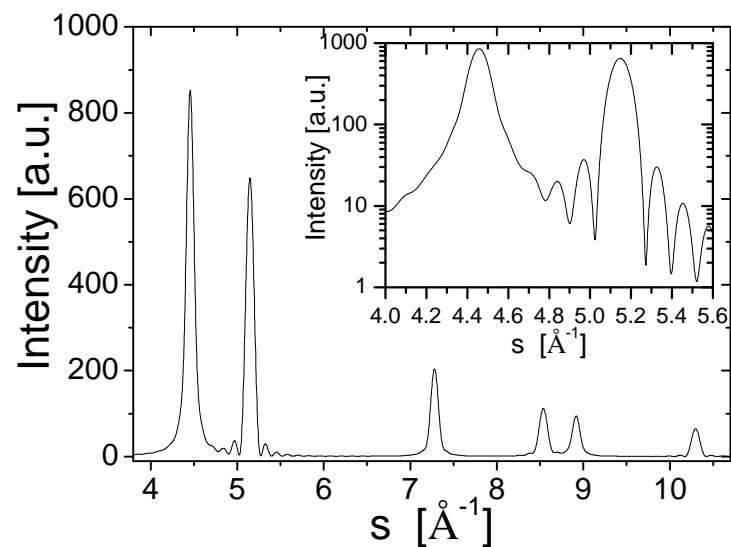
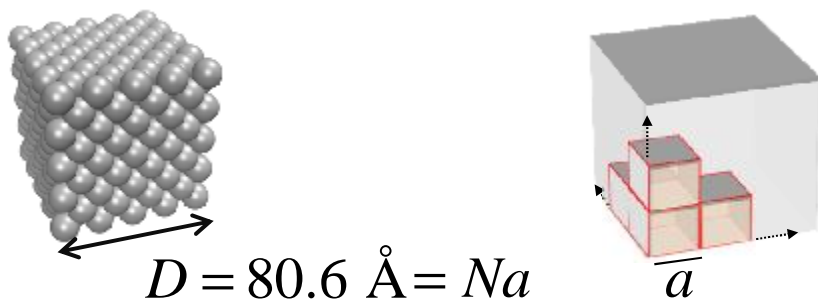


Courtesy of A. Young & F. Tsung
Boston College,
2015



IDEAL vs REAL NANOCRYSTALS

Microstructure: any deviation from perfect crystalline order



$$I_{PD}(s) \propto |F|^2 \Phi_{cube}(s, D)$$

Pd nanocrystals

Solla-Gullon et al., J. Appl. Cryst. 48 (2015). In press.

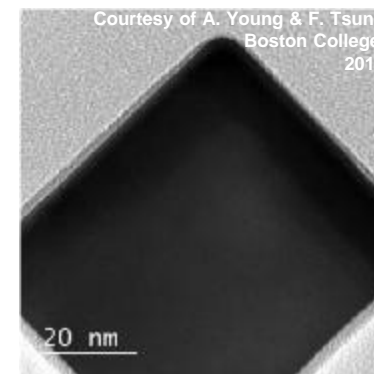
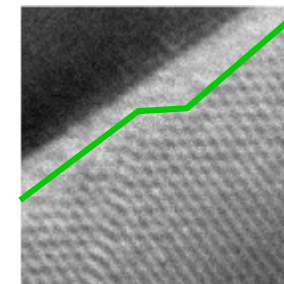
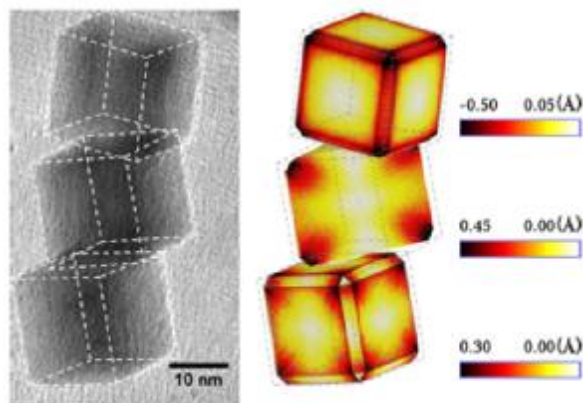
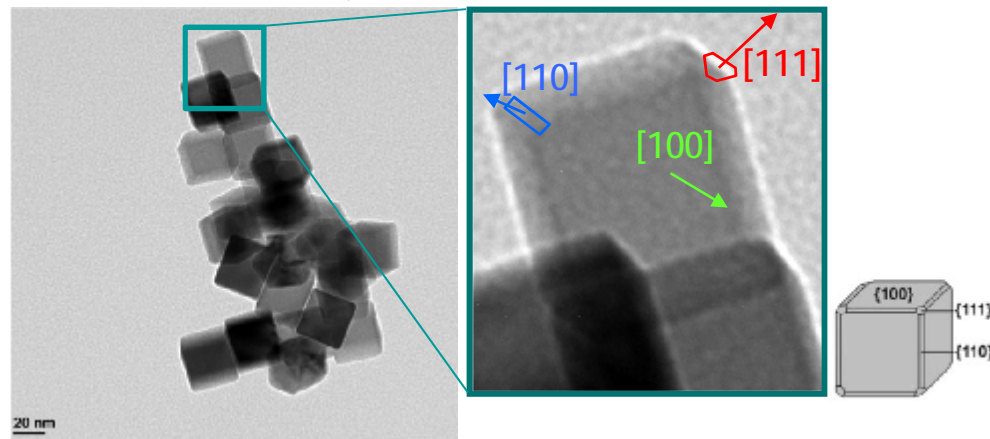


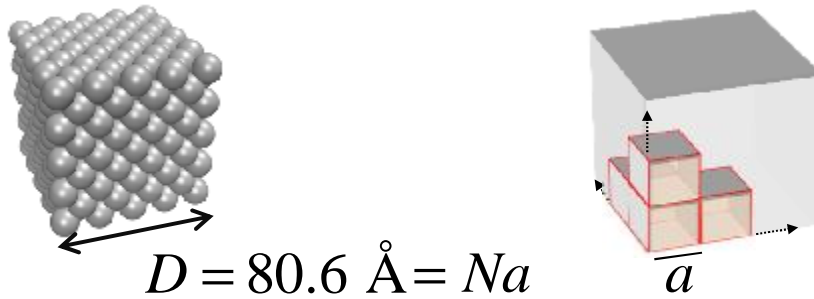
FIG. 6. (Color online) TEM picture of Pd nanocubes (left, dash is drawn just to drive the eye) with corresponding atomic displacement maps (right) for: normal component on the surface (top), norm of the component projected on the (110) cross section (middle), and on the surface of the nanocrystal (bottom).

Scardi et al., Phys.Rev. B 91 (2015) 155414

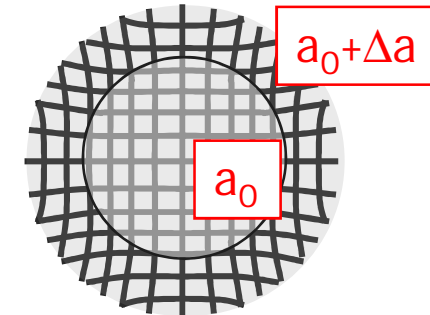
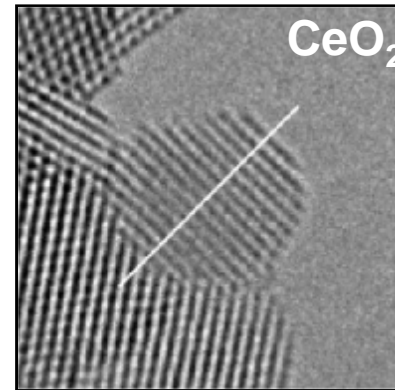
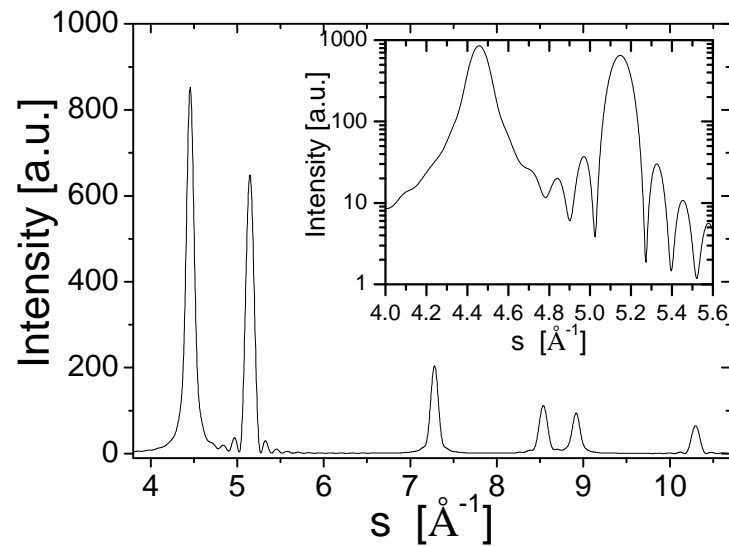
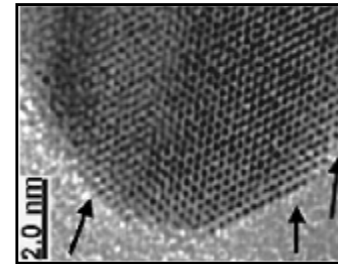


IDEAL vs REAL NANOCRYSTALS

Microstructure: any deviation from perfect crystalline order



Surface relaxation in nanocrystals

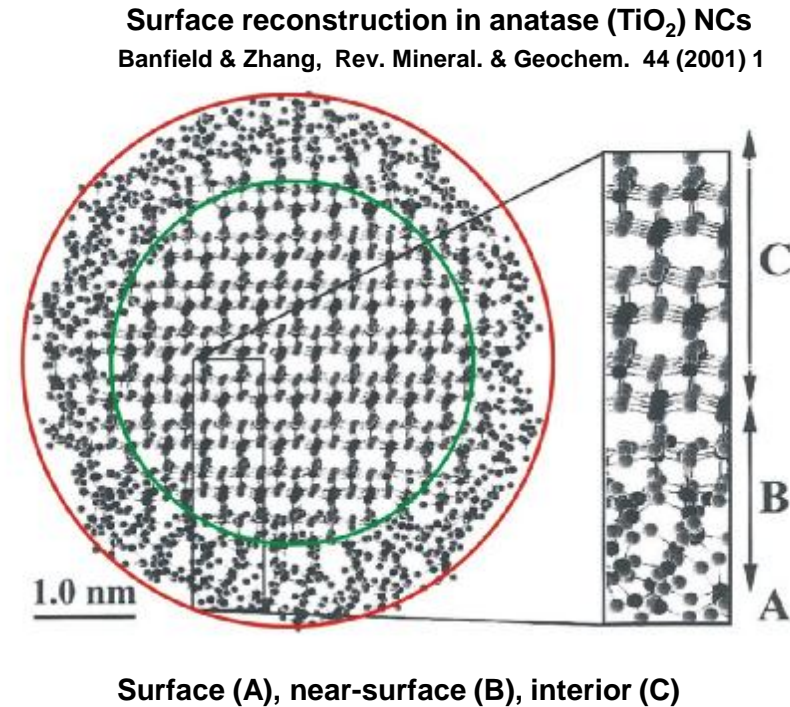
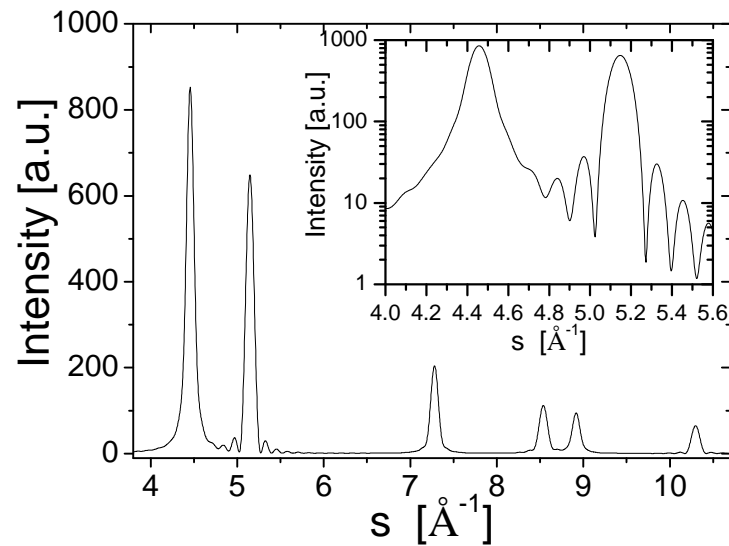
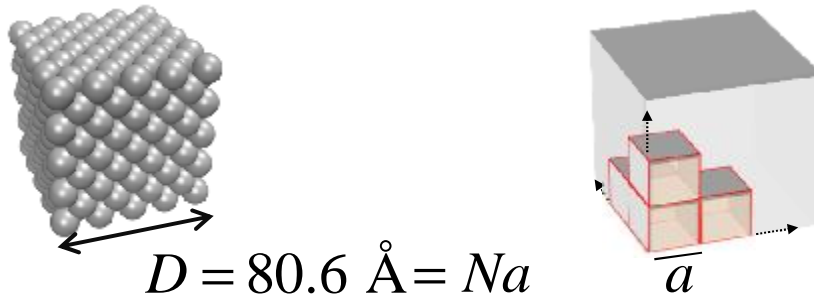


$$I_{PD}(s) \propto |F|^2 \Phi_{cube}(s, D)$$



IDEAL vs REAL NANOCRYSTALS

Microstructure: any deviation from perfect crystalline order

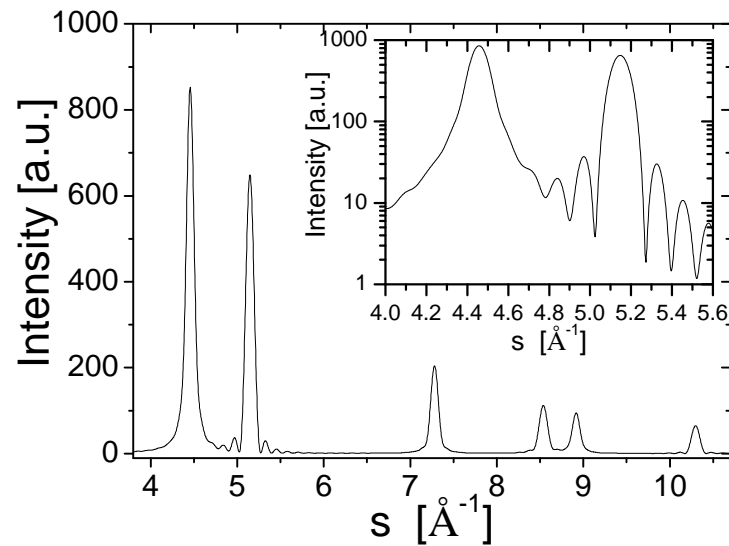
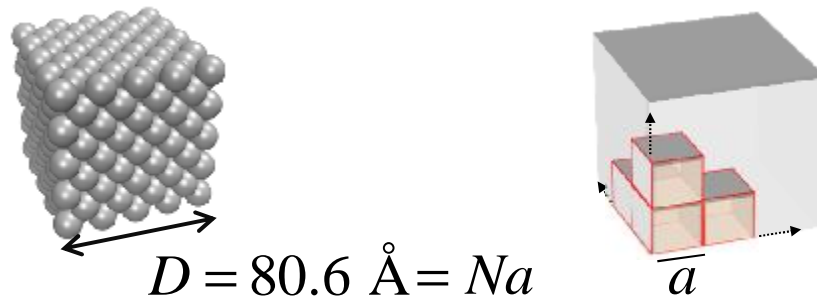


$$I_{PD}(s) \propto |F|^2 \Phi_{cube}(s, D)$$



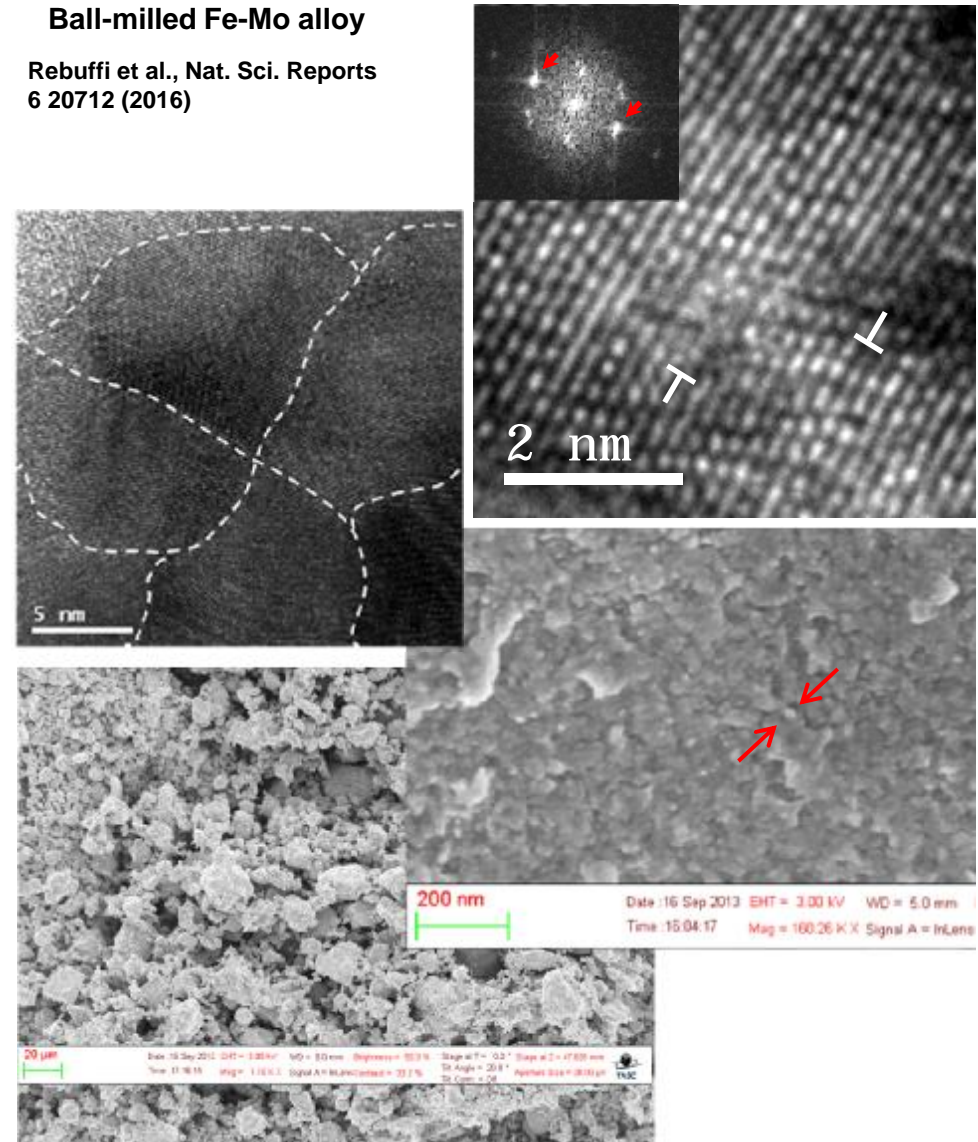
IDEAL vs REAL NANOCRYSTALS

Microstructure: any deviation from perfect crystalline order



$$I_{PD}(s) \propto |F|^2 \Phi_{cube}(s, D)$$

Ball-milled Fe-Mo alloy
Rebuffi et al., Nat. Sci. Reports
6 20712 (2016)





DIFFRACTION PATTERN FROM A POLYCRYSTALLINE

Experimental peak profiles (h) can be represented as a convolution :

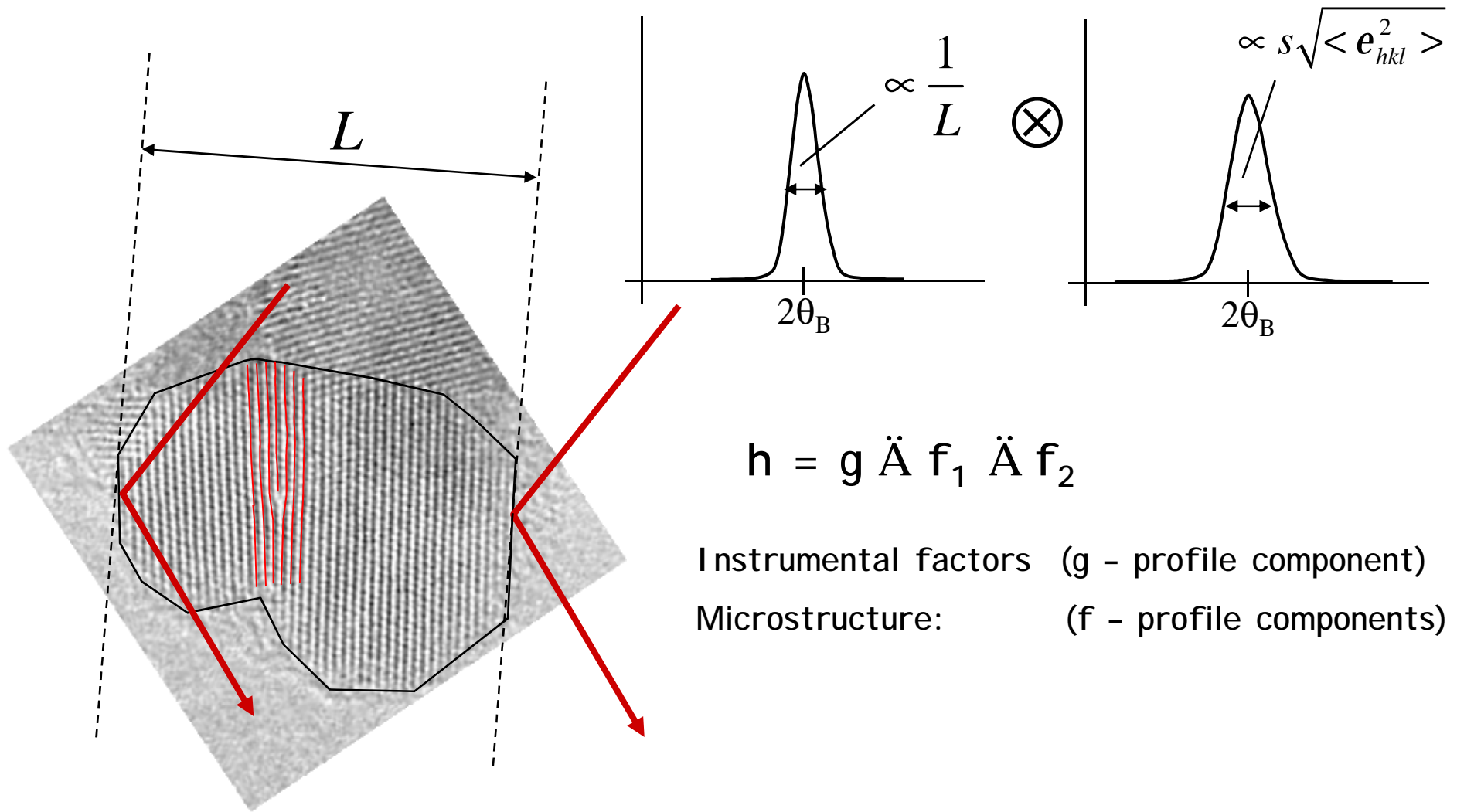
$$h = g \otimes f_1 \otimes f_2 \otimes f_3 \otimes \dots$$

- ∅ Instrumental factors: (g - profile component)
- ∅ Microstructure: (f - profile components)



DIFFRACTION PATTERN FROM A POLYCRYSTALLINE

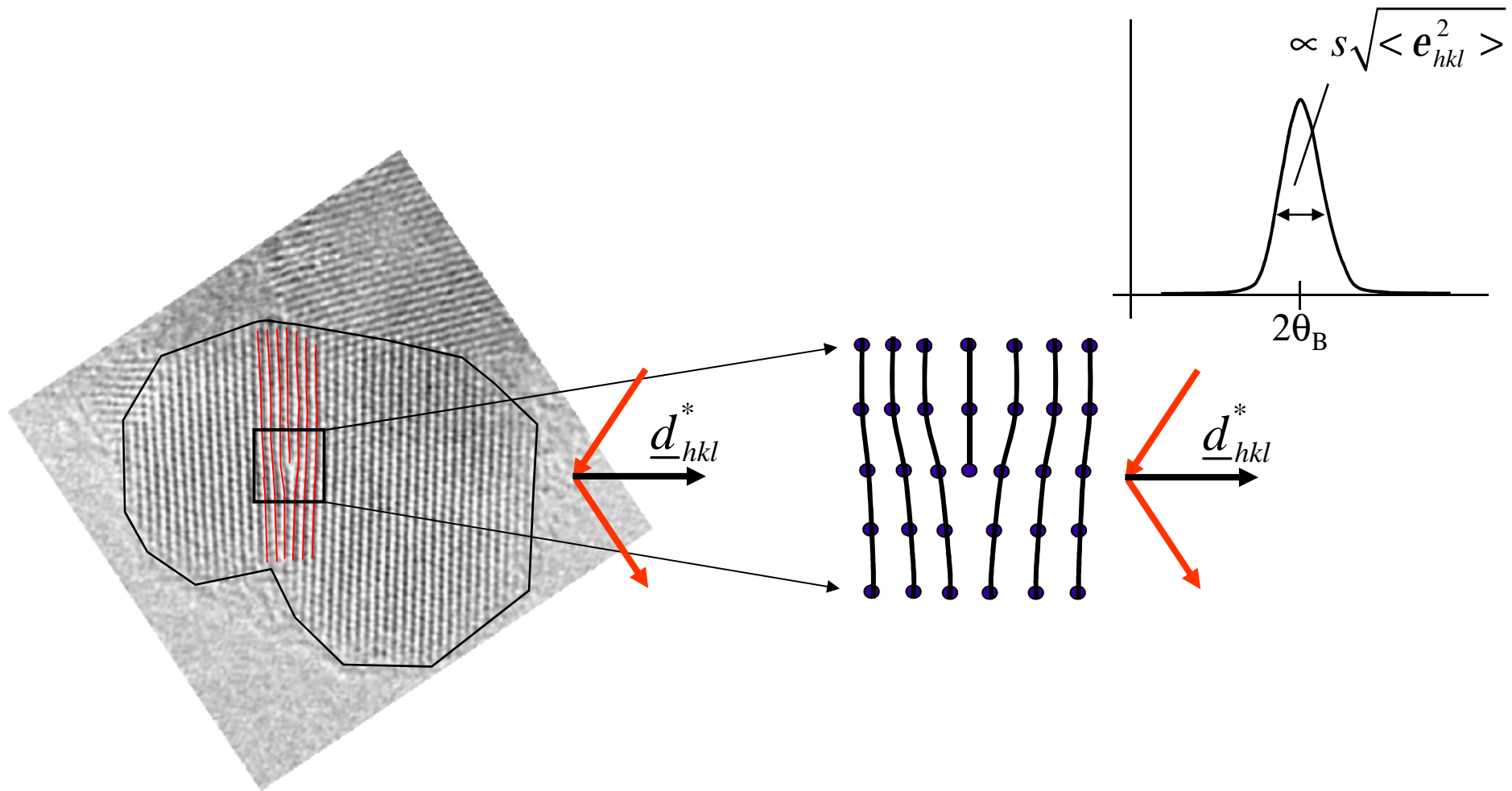
line broadening from instrument, domain size/shape and dislocations





DOMAIN SIZE AND MICROSTRAIN BROADENING

Dislocation line broadening is markedly anisotropic, i.e., hkl dependent

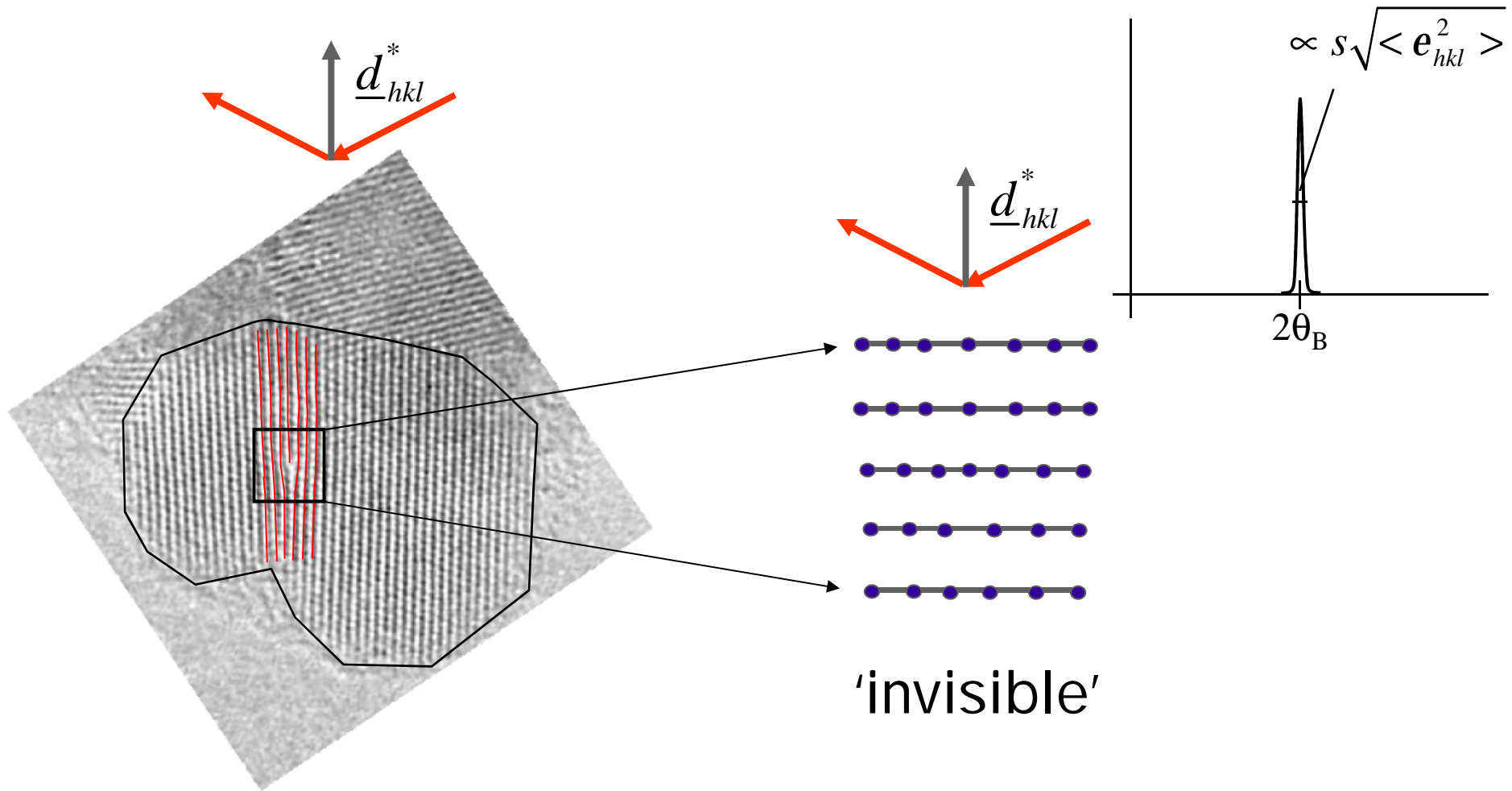


dislocation visibility depends on the viewing direction



DOMAIN SIZE AND MICROSTRAIN BROADENING

Dislocation line broadening is markedly anisotropic, i.e., hkl dependent

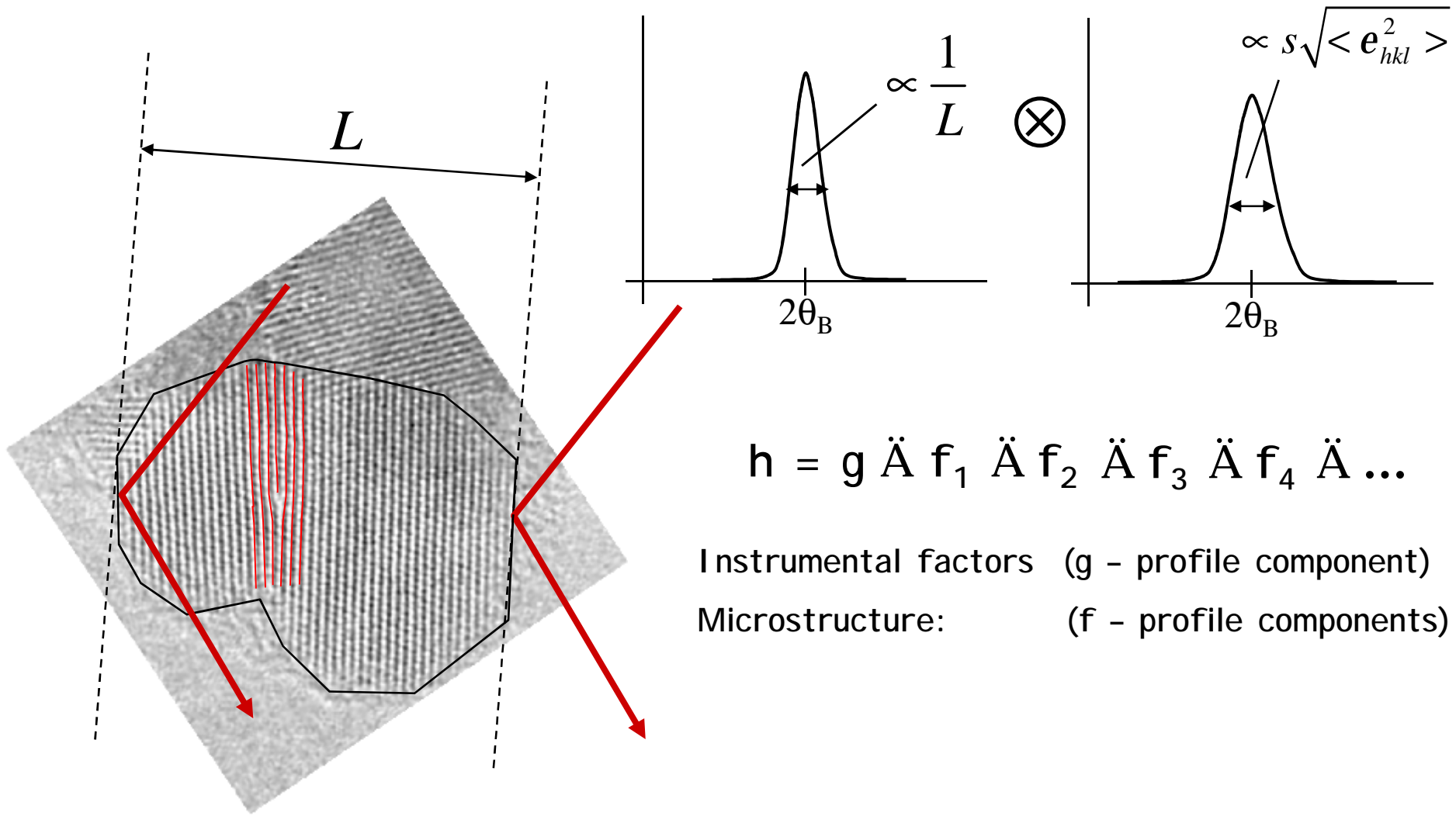


dislocation visibility depends on the viewing direction



DOMAIN SIZE AND MICROSTRAIN BROADENING

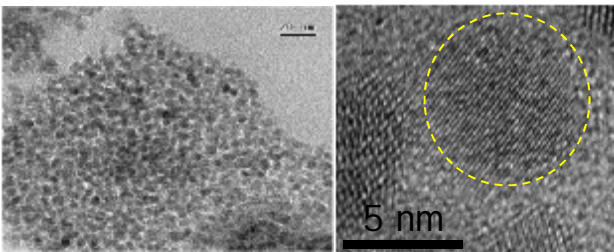
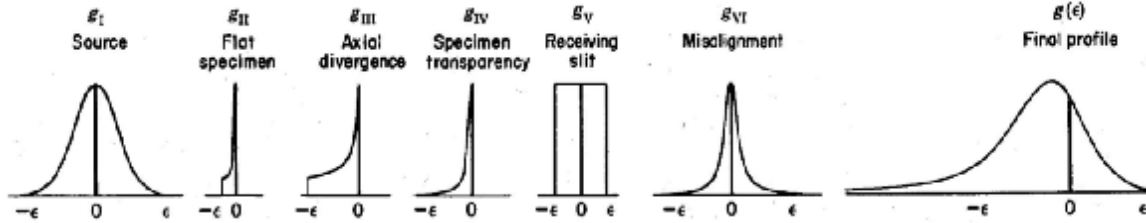
Combined line broadening effect from domain size and dislocations



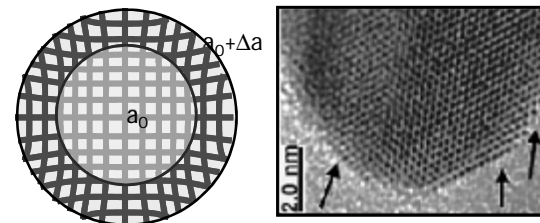
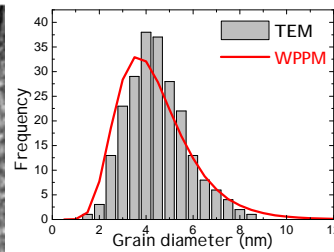


DIFFRACTION PATTERN FROM A POLYCRYSTALLINE

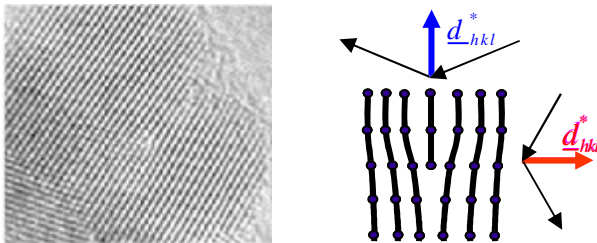
Most common line broadening sources



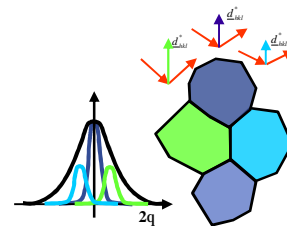
Grain shape and size distribution



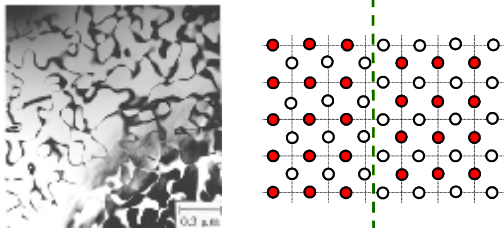
Grain surface relaxation



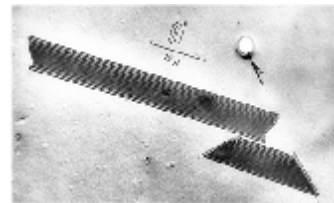
dislocations, disclinations



stoichiometry fluctuation



Anti-phase boundaries



Stacking faults

g

$f_1 \otimes f_2 \otimes f_3 \otimes \dots$



WHOLE POWDER PATTERN MODELLING

Diffraction profile as a convolution of (independent) effects:

$$I(s) = I^{IP}(s) \otimes I^S(s) \otimes I^D(s) \otimes I^F(s) \otimes I^{APB}(s) \otimes \dots$$

the Fourier Transform of $I(s)$ is the product of the FTs of the single profile components

$$I(s) \propto \int_{-\infty}^{\infty} C(L) e^{2\pi i L \cdot s_{hkl}} dL$$

$$C = \prod_i A_i = T_{pV}^{IP} \cdot A_{\{hkl\}}^S \cdot A_{\{hkl\}}^D \cdot (A_{hkl}^F + iB_{hkl}^F) \cdot A_{\{hkl\}}^{APB} \cdot \dots$$

instr. profile domain size/shape microstrain / lattice defects/...

P. Scardi, Chap. 13 in Powder Diffraction: Theory and Practice, R.E. Dinnebier & S.J.L. Billinge, eds. RSC, Cambridge, 2008

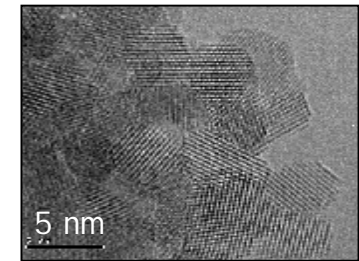
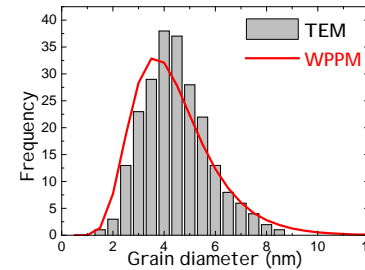


WPPM : HOW DOES IT WORK ??

$$T_{pV}^{IP}(L) = (1-k) \cdot \exp(-p^2 \cdot s_s^2 L^2 / \ln 2) + k \exp(-2p \cdot s_s L) \quad \text{Instrumental profile}$$

Domain size effect: m, s

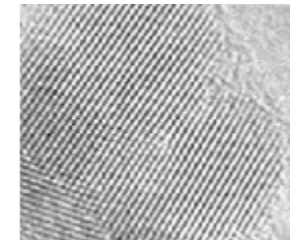
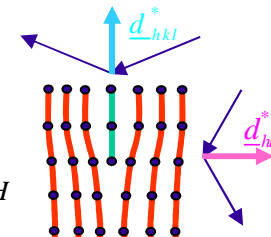
$$A^S(L) = \sum_{n=0}^3 H_n^c \cdot \text{Erfc} \left[\frac{\ln(L \cdot K^c) - m - (3-n)s^2}{s\sqrt{2}} \right] \frac{M_{l,3-n}}{2M_{l,3}} \cdot L^n$$



Dislocation (strain) effect: $r, Re, (\bar{C}_{hkl})$

$$A_{\{hkl\}}^D(L) = \exp \left[-\frac{1}{2} p |b|^2 \bar{C}_{hkl} r d_{\{hkl\}}^{*2} \cdot L^2 f^*(L/R_e) \right]$$

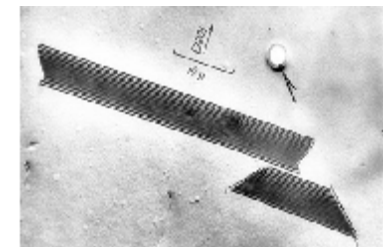
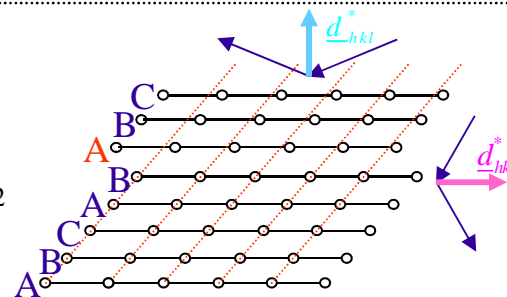
$$\bar{C}_{hkl} = A + B \cdot \frac{h^2 k^2 + k^2 l^2 + l^2 h^2}{(h^2 + k^2 + l^2)^2} = A + B \cdot H$$



Faulting: a (def.), b (twin)

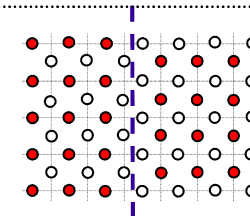
$$A_{hkl}^F(L) = (1 - 3a - 2b + 3a^2) \left| \frac{1}{2} L d_{\{hkl\}}^* \frac{L_0}{h_0^2} s_{L_0} \right|$$

$$B_{hkl}^F(L) = -s_{L_0} \cdot \frac{L}{|L|} \cdot \frac{L_0}{|L_0|} \cdot b / (3 - 6b - 12a - b^2 + 12a^2)^{1/2}$$



Anti-Phase Domains: g

$$A_{\{hkl\}}^{APB}(L) = \exp \left[-\frac{2g (|h| + |k|) \cdot L}{d_{hkl} (h^2 + k^2 + l^2)} \right]$$





WHOLE POWDER PATTERN MODELLING - WPPM

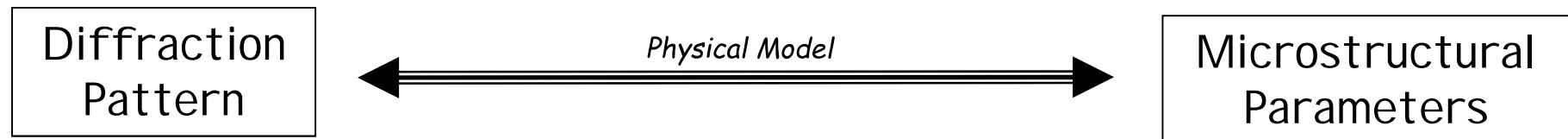
based on physical models of the microstructure

$$I(s) \propto \int_{-\infty}^{\infty} C(L) e^{2\pi i L \cdot s_{hkl}} dL$$

$$C = \prod_i A_i = T_{pV}^{IP} \cdot A_{\{hkl\}}^S \cdot A_{\{hkl\}}^D \cdot (A_{hkl}^F + iB_{hkl}^F) \cdot A_{\{hkl\}}^{APB} \cdot \dots$$

instr. profile
domain size/shape
microstrain / lattice defects/...

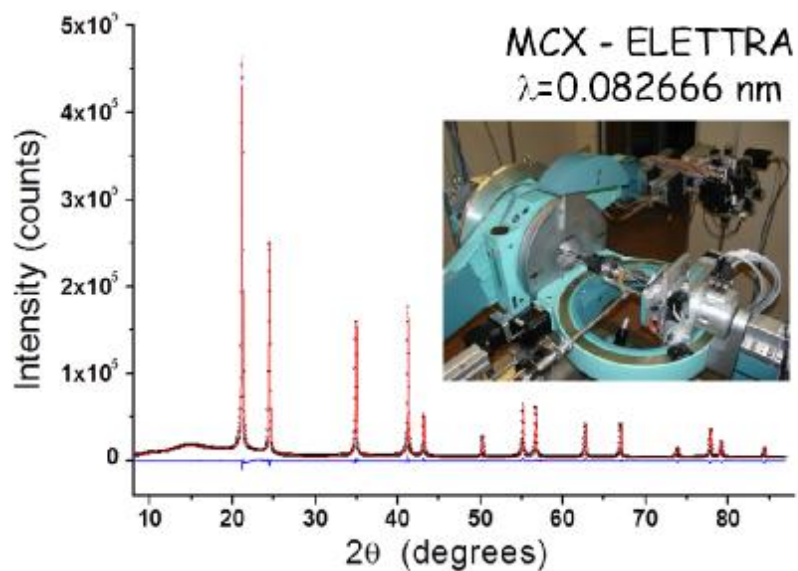
Direct modelling of diffraction profiles in terms of relatively few microstructural parameters: $m, s - r, R_e - a, b - g \dots$



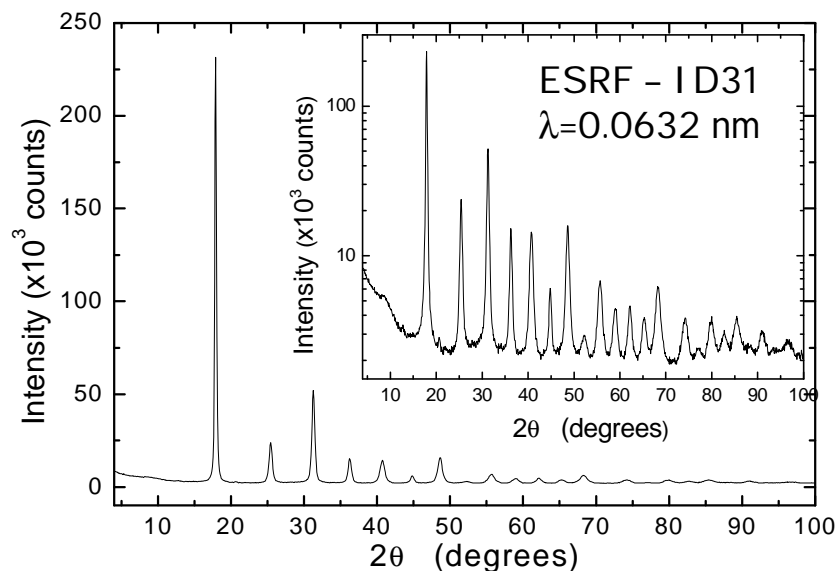
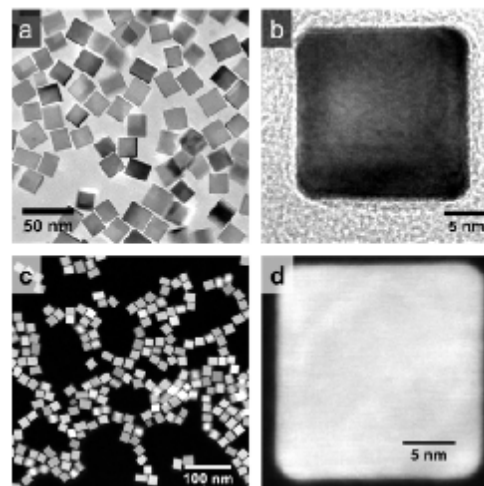
P. Scardi, Chap. 13 in Powder Diffraction: Theory and Practice, R.E. Dinnebier & S.J.L. Billinge, eds. RSC, Cambridge, 2008



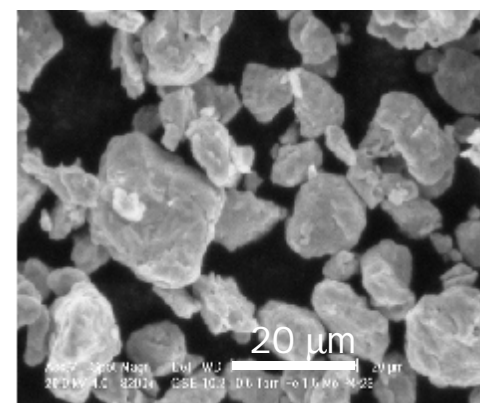
WPPM APPLICATIONS: TWO TYPICAL CASES OF STUDY



"identical" Pd nanoparticles



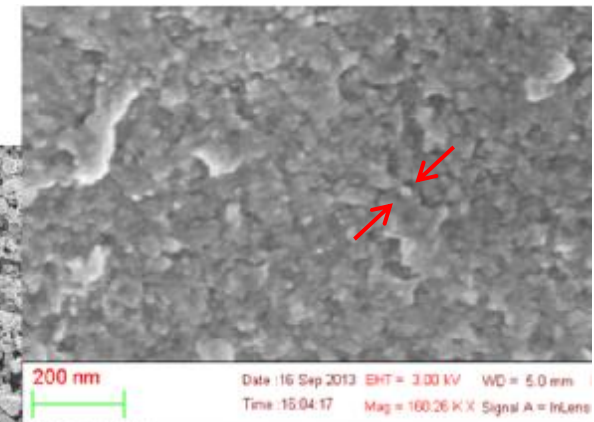
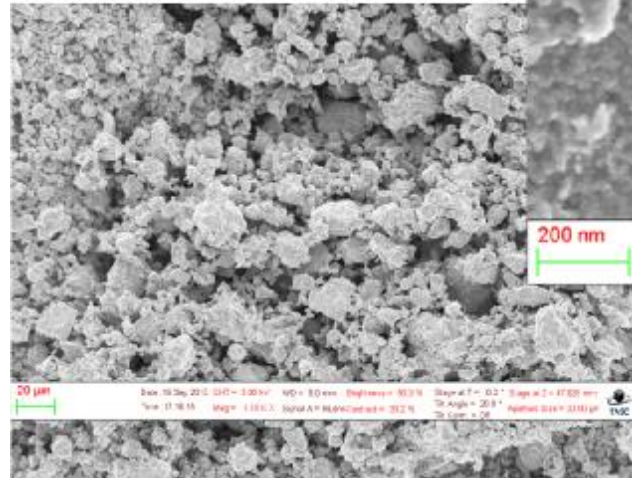
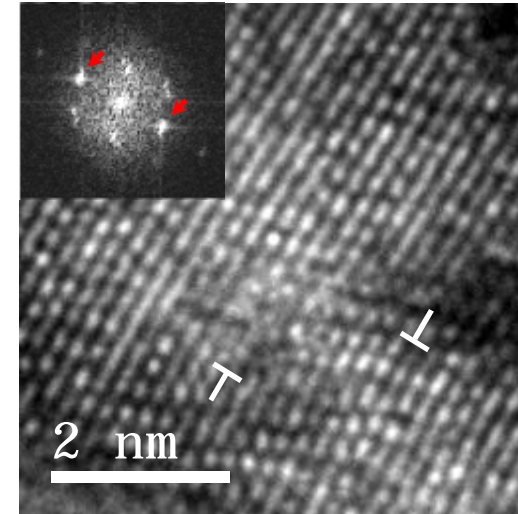
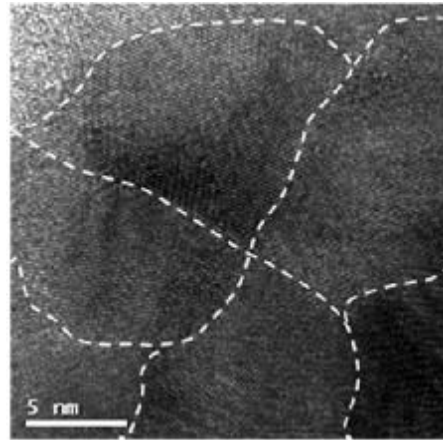
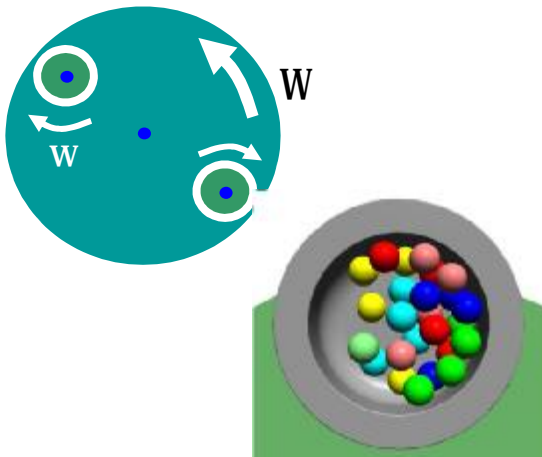
Ball milled Fe-1.5%Mo





NANOCRYSTALLINE Fe-1.5%Mo POWDER

Planetary ball milling - production of nanocrystalline Fe-1.5%Mo



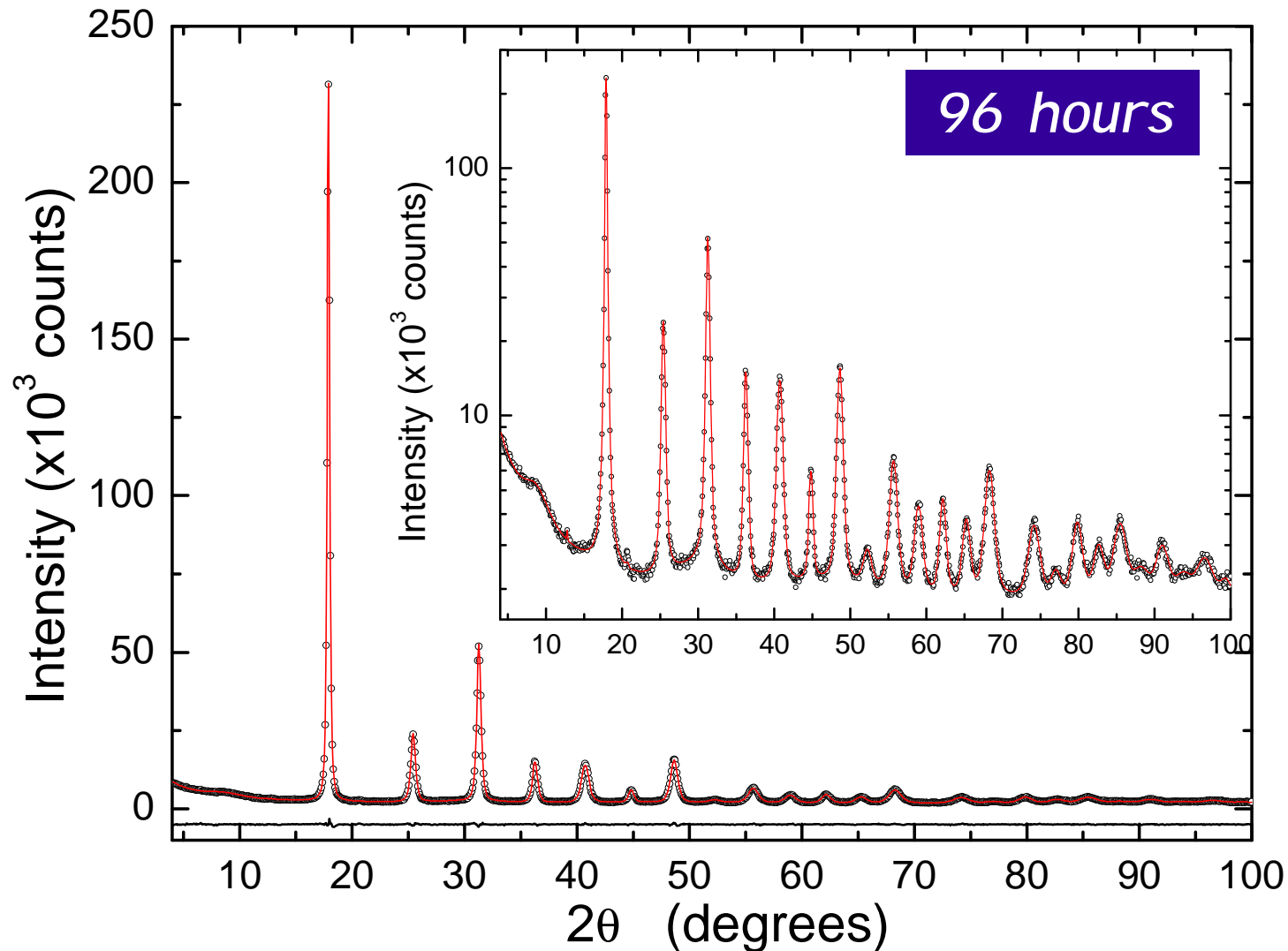
Rebuffi et al., Nat. Sci. Reports 6 20712 (2016)

P. Scardi - Diffraction from nanocrystalline materials



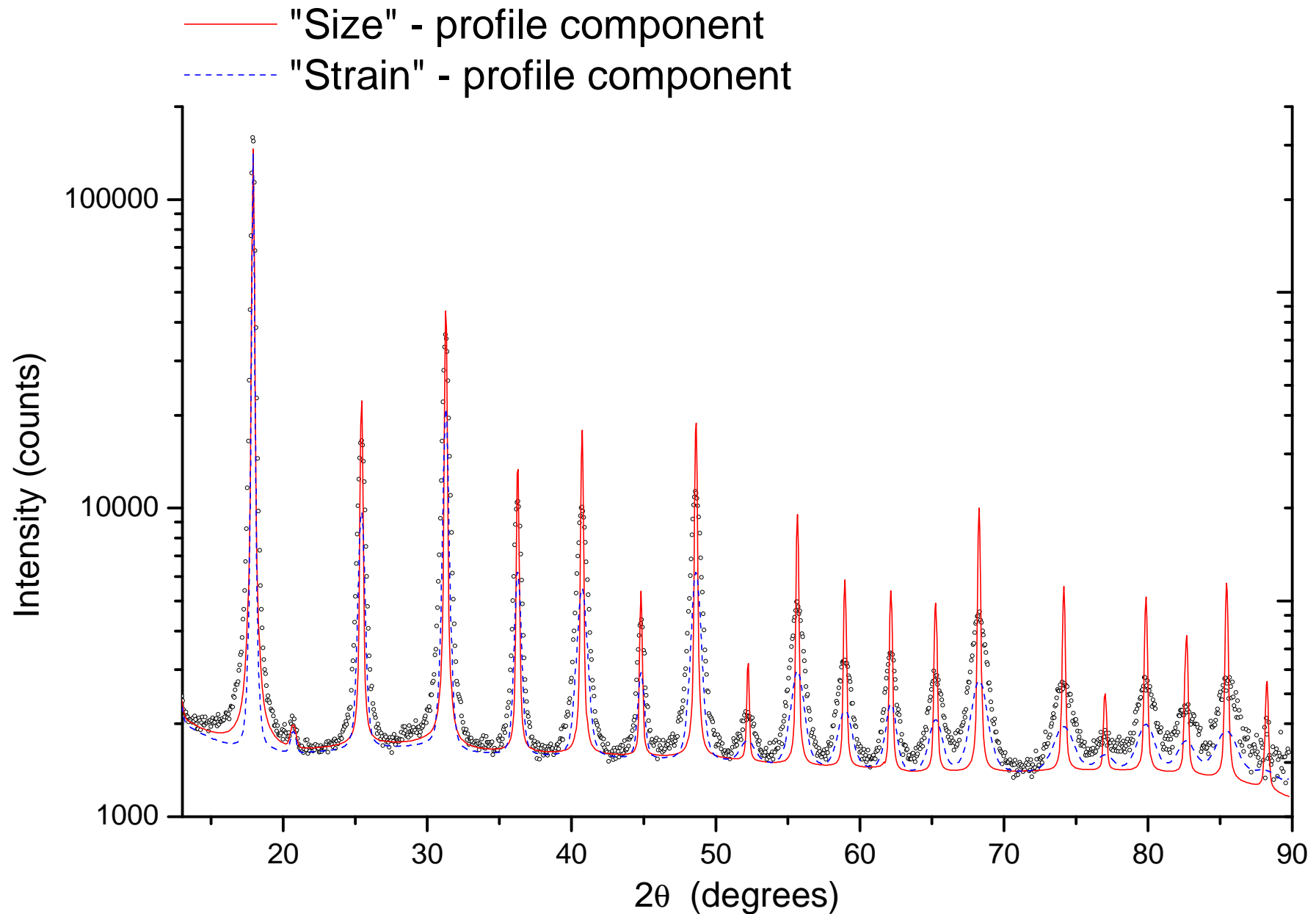
NANOCRYSTALLINE Fe-1.5%Mo POWDER

Ball milled Fe1.5Mo (Fritsch P4) - data collected at ESRF - ID31 $\lambda=0.0632$ nm



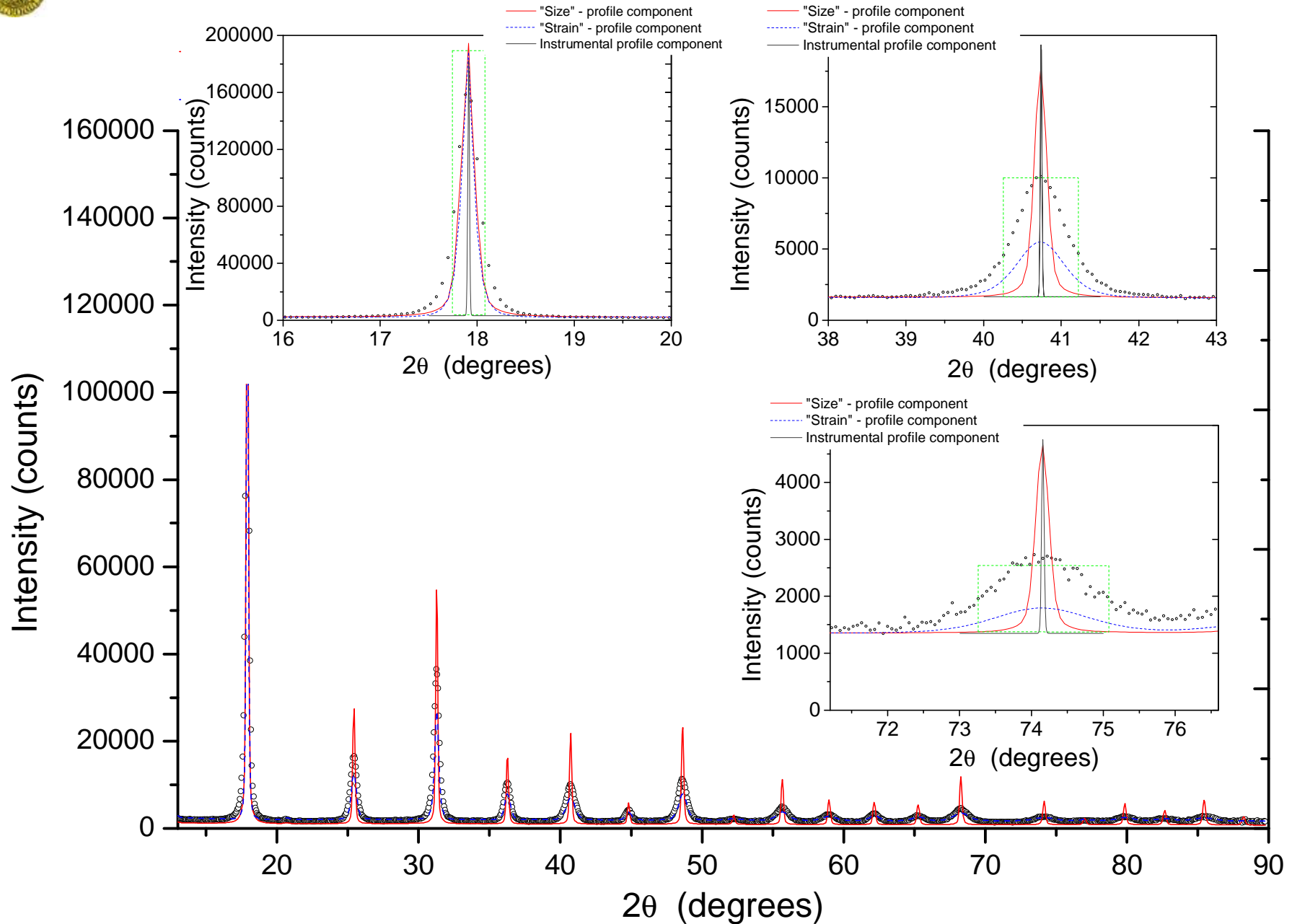


SIZE AND MICROSTRAIN PROFILE COMPONENTS



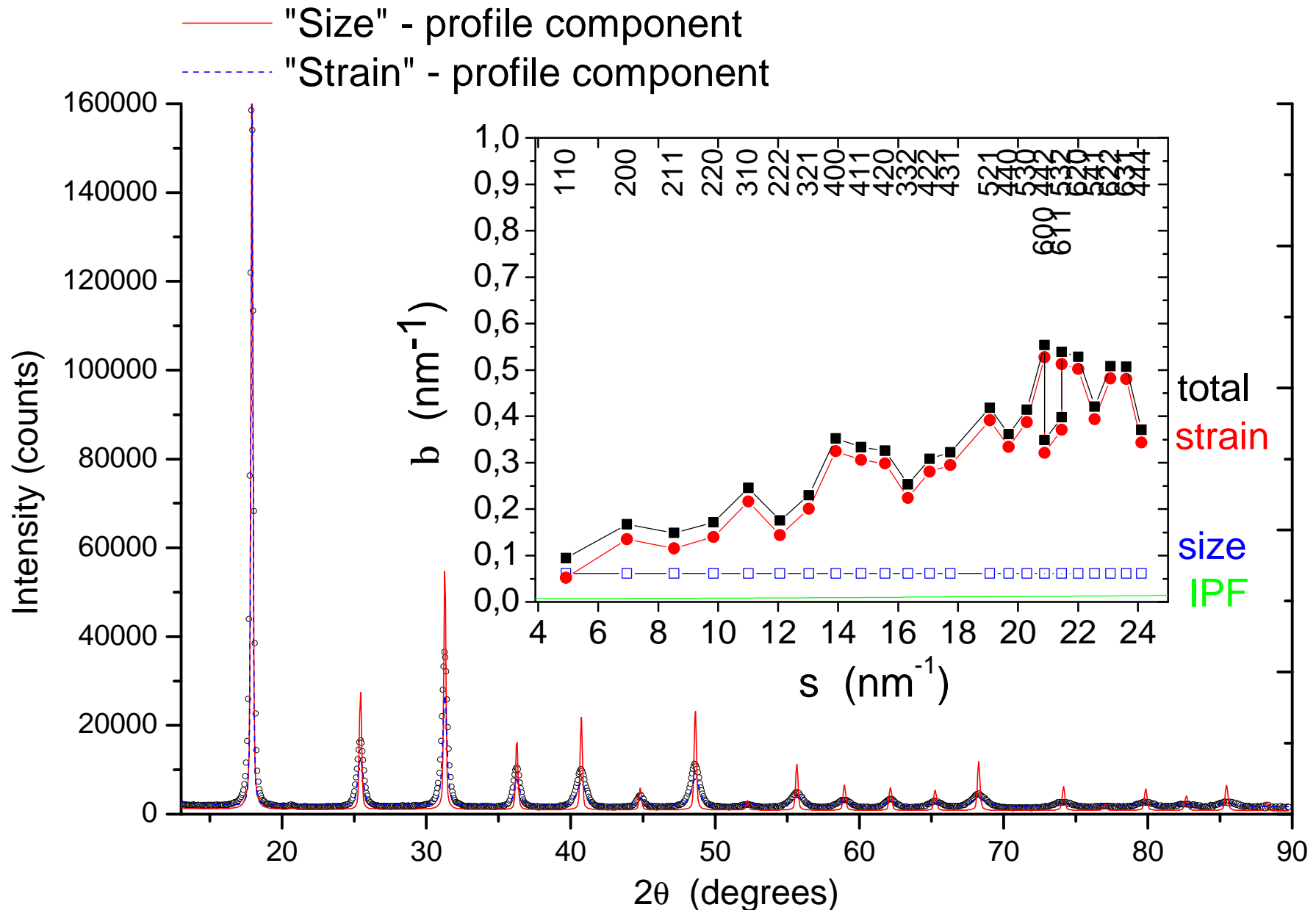


SIZE AND MICROSTRAIN PROFILE COMPONENTS





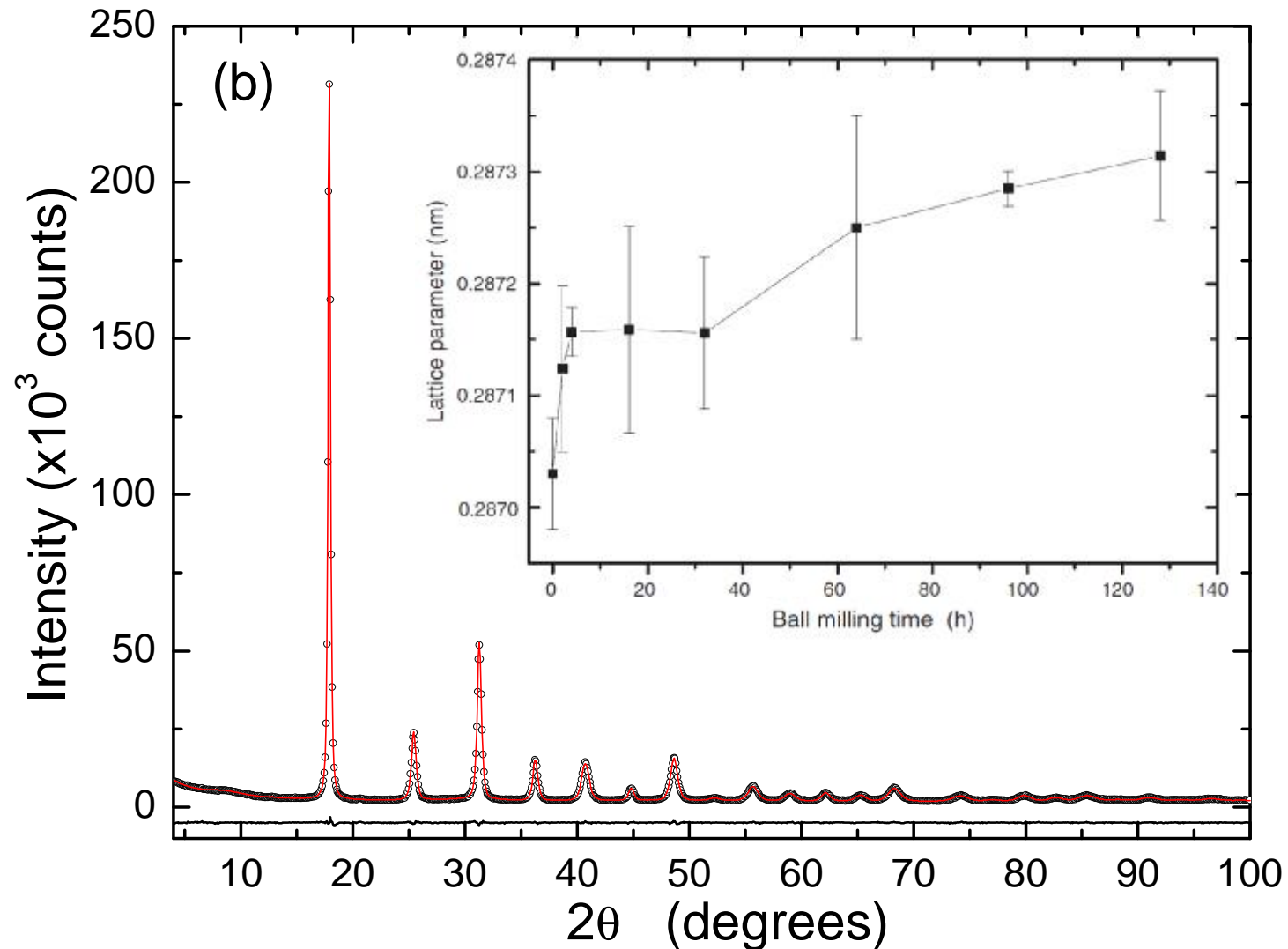
SIZE AND MICROSTRAIN PROFILE COMPONENTS





NANOCRYSTALLINE Fe-1.5%Mo POWDER

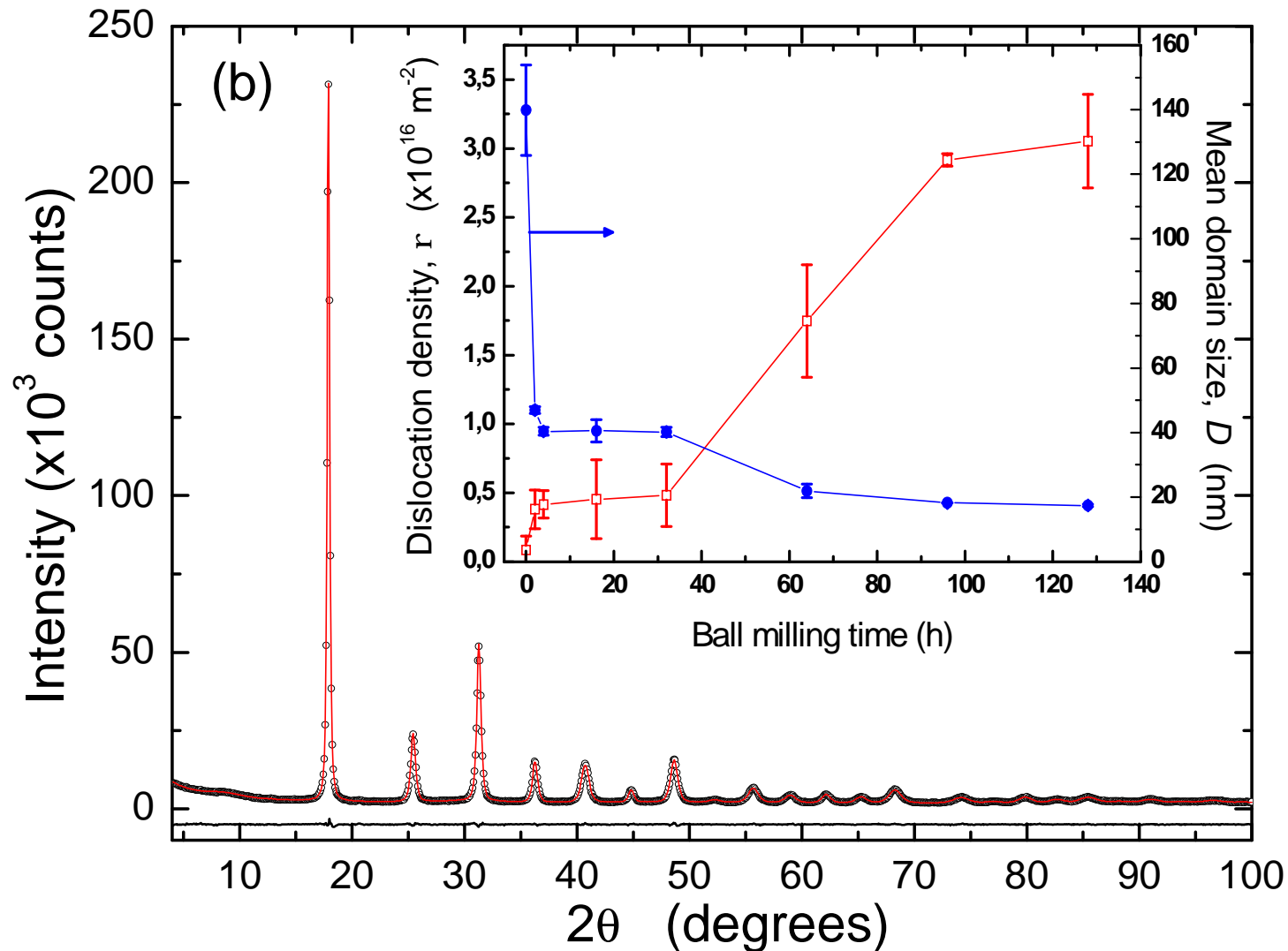
Ball milled Fe1.5Mo (Fritsch P4) - data collected at ESRF - ID31 $\lambda=0.0632$ nm





NANOCRYSTALLINE Fe-1.5%Mo POWDER

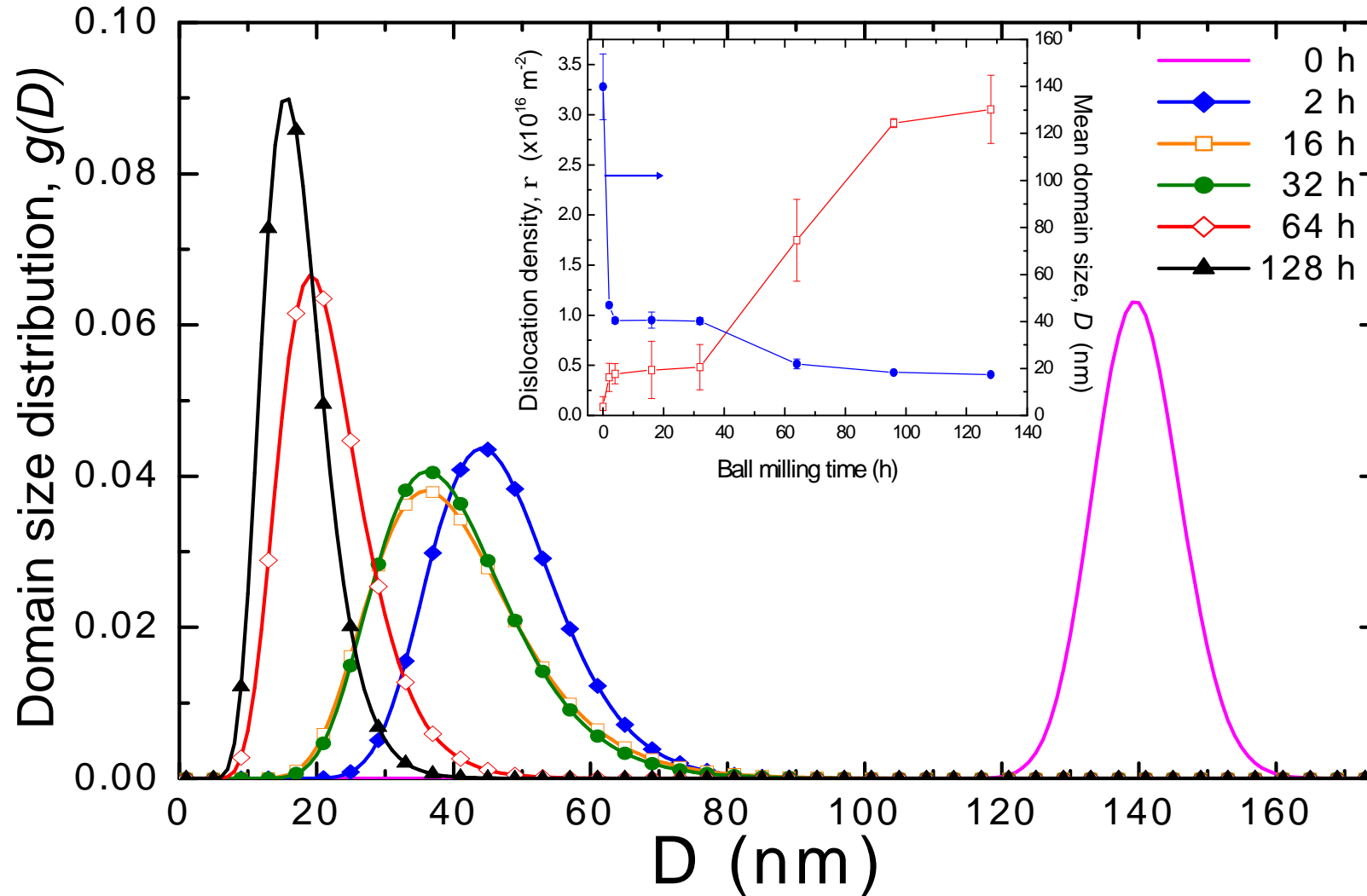
Ball milled Fe1.5Mo (Fritsch P4) - data collected at ESRF - ID31 $\lambda=0.0632$ nm





NANOCRYSTALLINE Fe-1.5%Mo POWDER

Ball milled Fe1.5Mo (Fritsch P4) – data collected at ESRF – ID31 $\lambda=0.0632$ nm
In addition to mean values, WPPM provides the size distribution



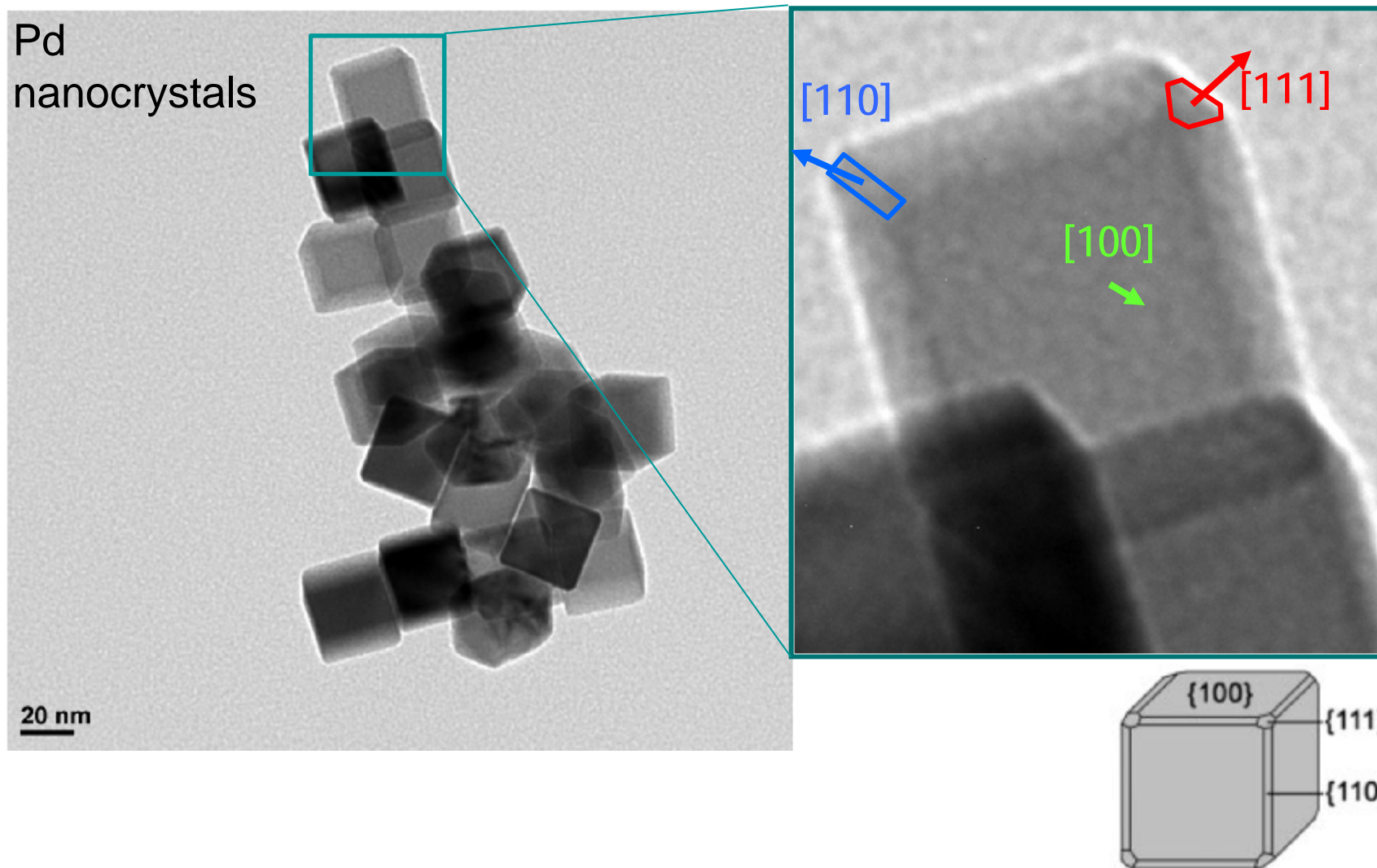
Rebuffi et al., Nat. Sci. Reports 6 20712 (2016) - open access – and references therein



CHALLENGES IN NANOTECHNOLOGY

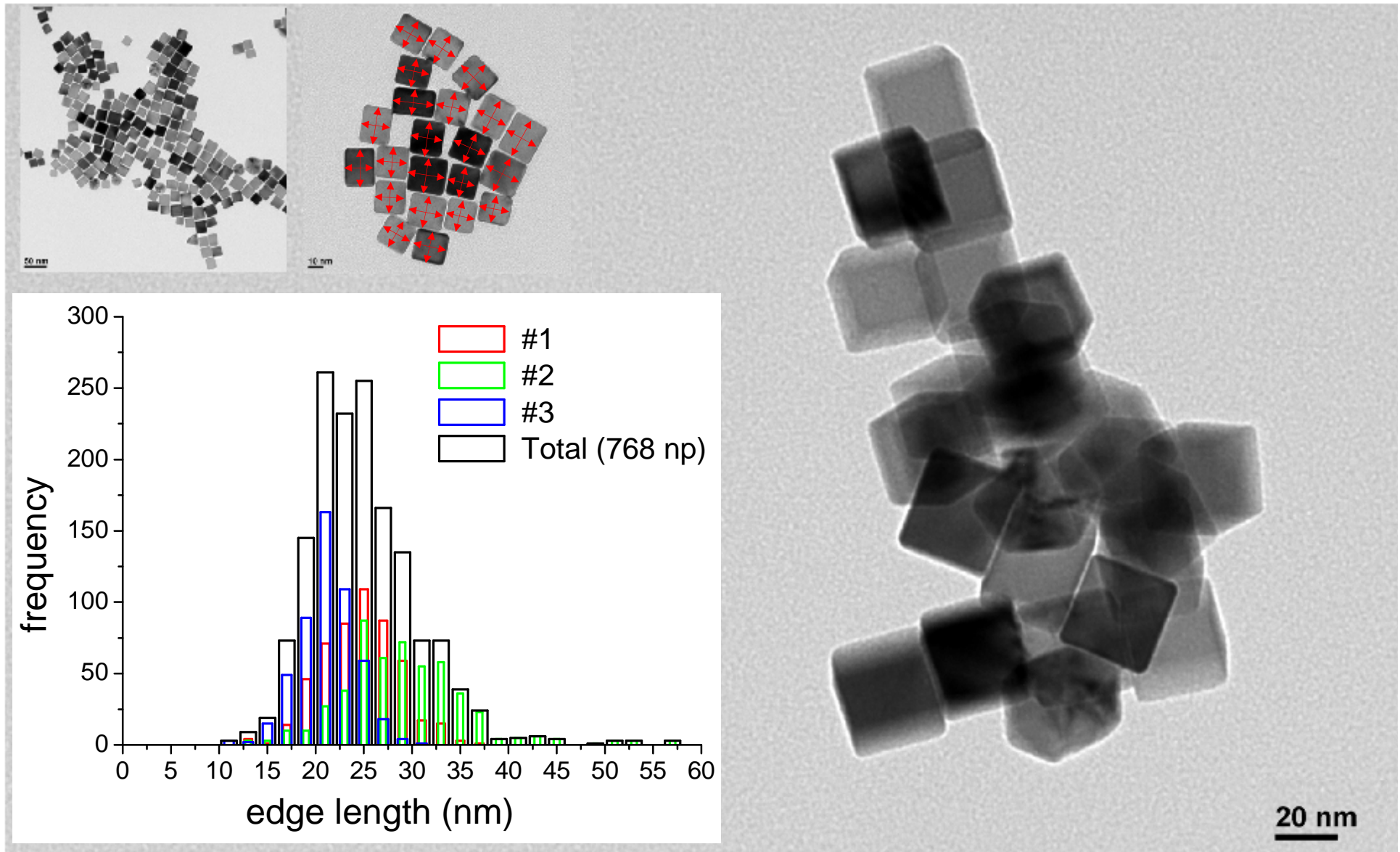
Production of “identical” nanoparticles. Nanocrystal size and shape:
X-ray Powder Diffraction and Transmission Electron Microscopy (TEM)

Solla Gullon et al., J. Appl. Cryst. 48 (2015) 1534





DIFFRACTION FROM NANOCRYSTALLINE POWDER

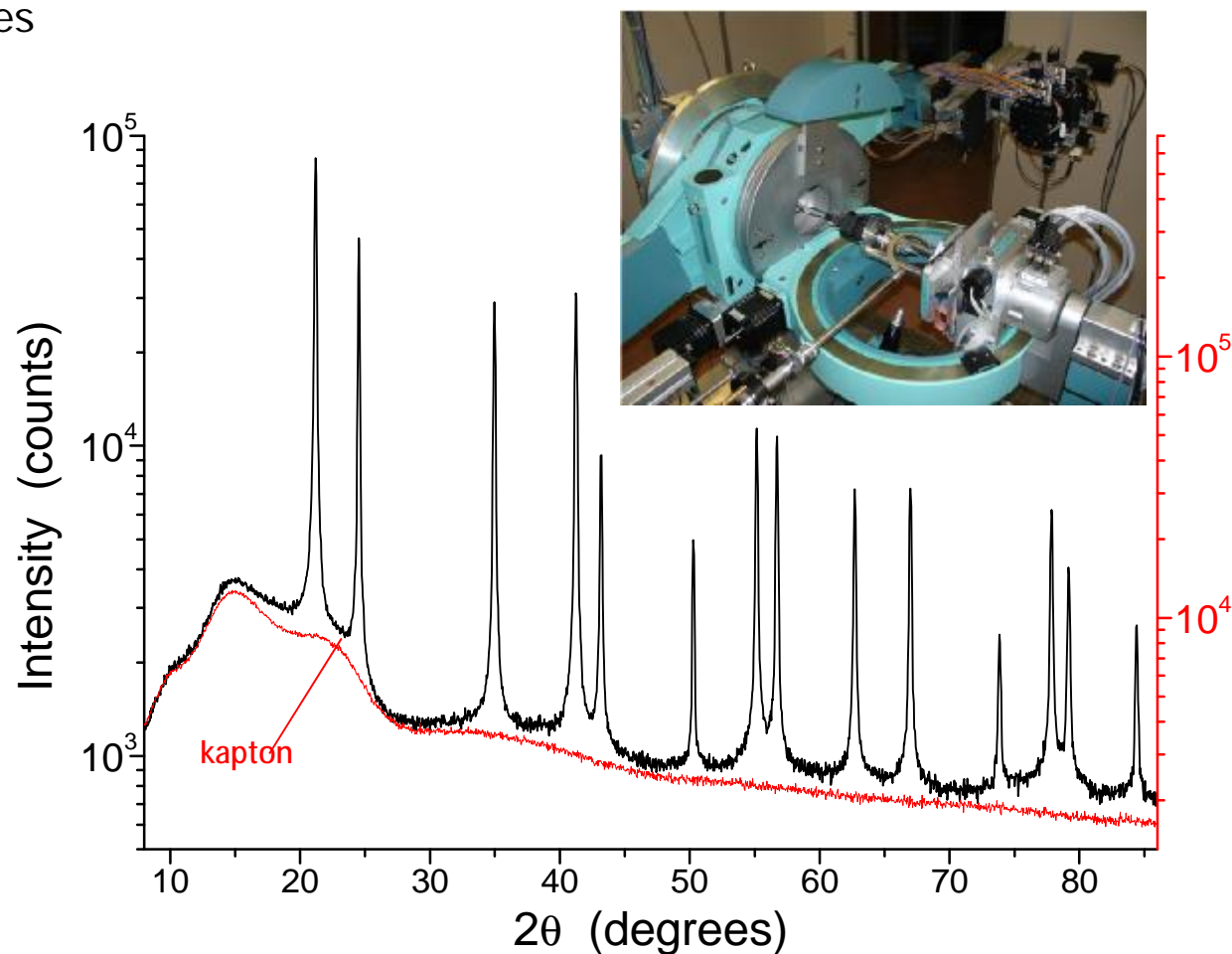




DIFFRACTION FROM NANOCRYSTALLINE POWDER

MCX beamline (Elettra Sincrotrone Trieste, Trieste)
Debye-Scherrer geometry, 15 keV, \varnothing 0.5 mm kapton capillary

- Ø Narrow instrumental profiles
- Ø Good counting statistics



Special thanks to: M. Abdellatief, L. Rebuffi, J. Plaisier, A. Lausi



DIFFRACTION FROM NANOCRYSTALLINE POWDER

MCX beamline (Elettra Sincrotrone Trieste, Trieste)
Debye-Scherrer geometry, 15 keV, Ø 0.5 mm kapton capillary

Ø Negligible absorption: $\mu=2.71 \text{ cm}^{-1} \Rightarrow \mu R \approx 0.07$

$$A(q, R, m) = \frac{1}{pR^2} \int_0^{2p} \int_0^R \exp \left\{ -m \left[\sqrt{R^2 - r^2 \sin^2(q+j)} + \sqrt{R^2 - r^2 \sin^2(q-j)} \right] \right\} \cosh(2mr \sin q \sin j) r dr dj$$

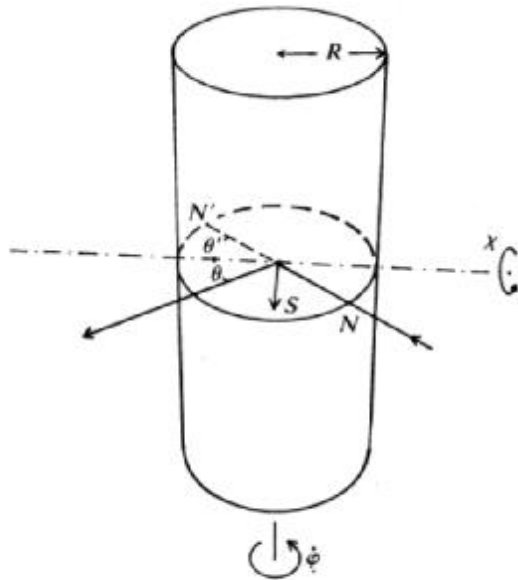
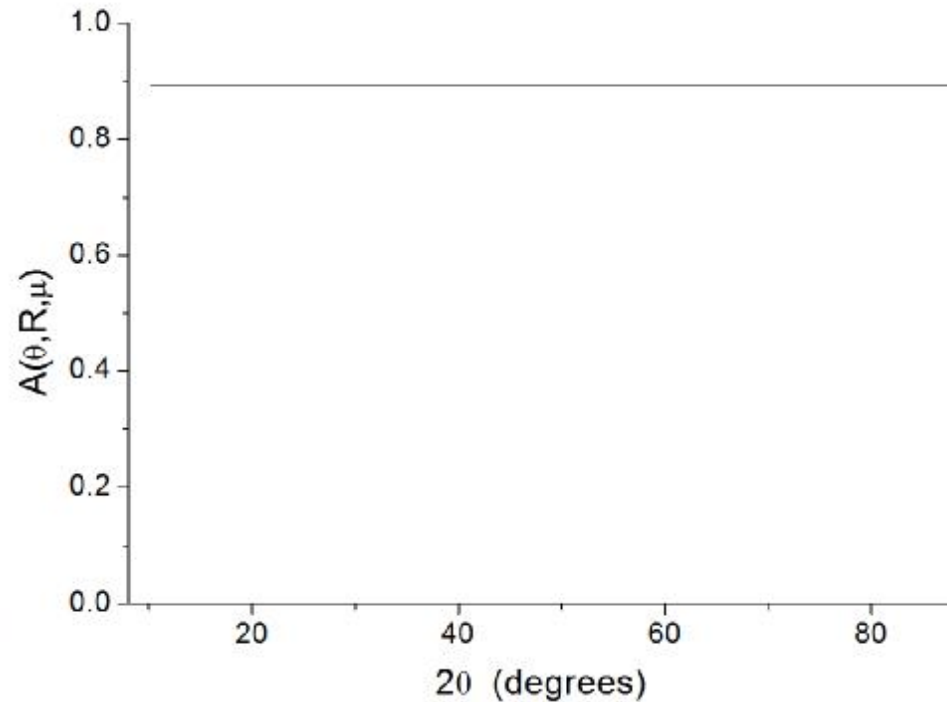


Fig. 6.3.3.1. Geometry of the Eulerian cradle with the axis of a cylindrical specimen coincident with the φ axis.

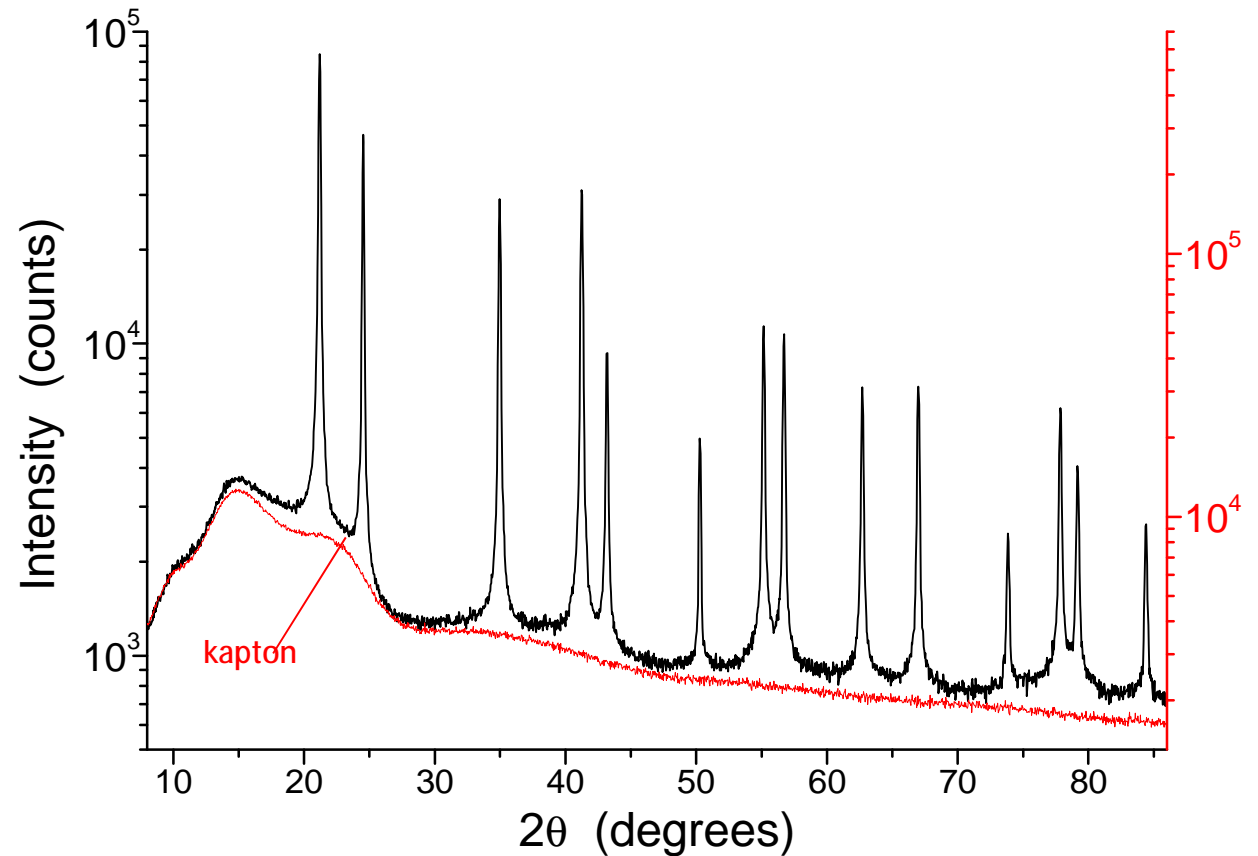




DIFFRACTION FROM NANOCRYSTALLINE *POWDER*

MCX beamline (Elettra Sincrotrone Trieste, Trieste)
Debye-Scherrer geometry, 15 keV, Ø 0.5 mm kapton capillary

Ø Carefully reproducible / controlled signal from the capillary

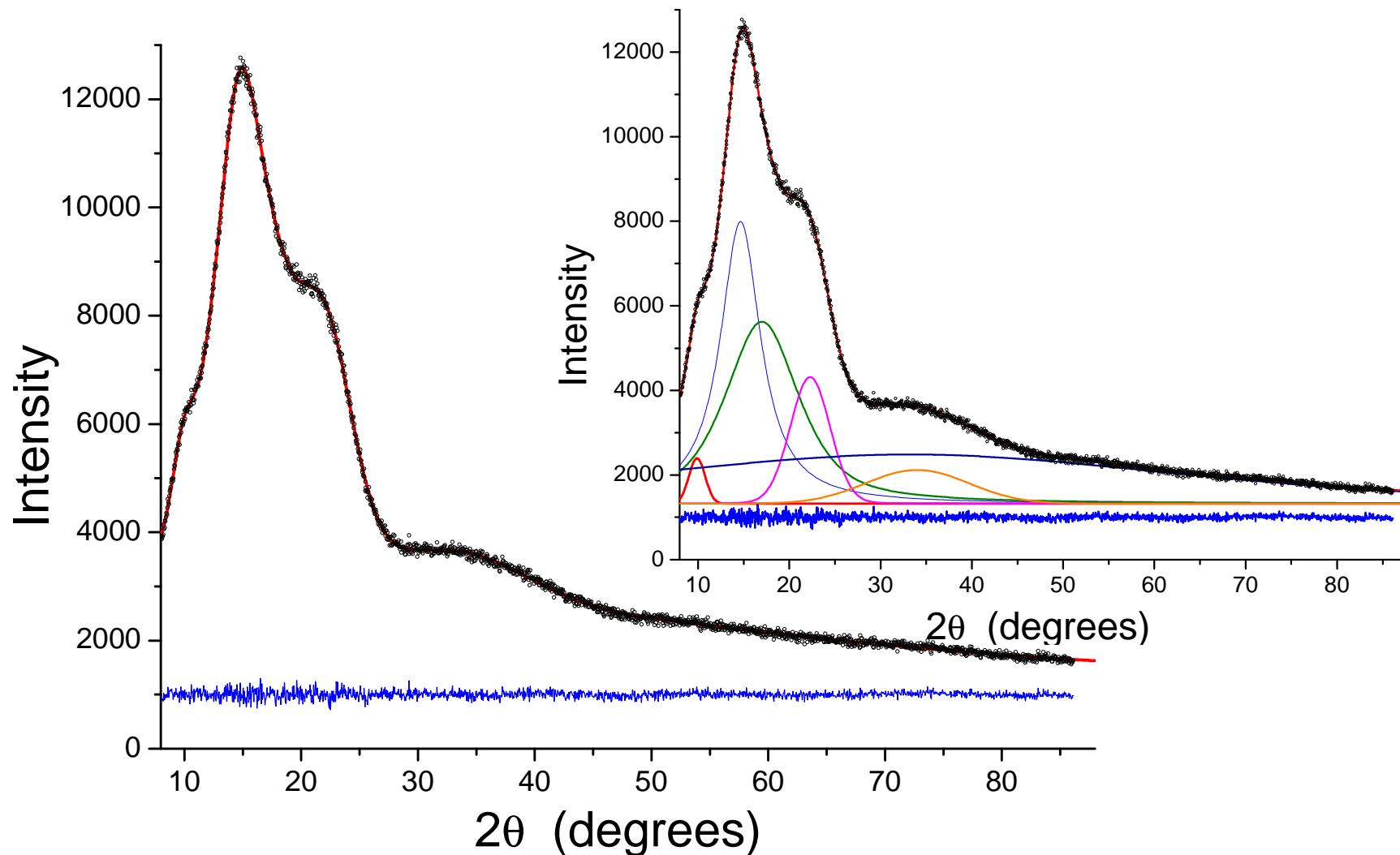




DIFFRACTION FROM NANOCRYSTALLINE POWDER

MCX beamline (Elettra Sincrotrone Trieste, Trieste)
Debye-Scherrer geometry, 15 keV, \varnothing 0.5 mm kapton capillary

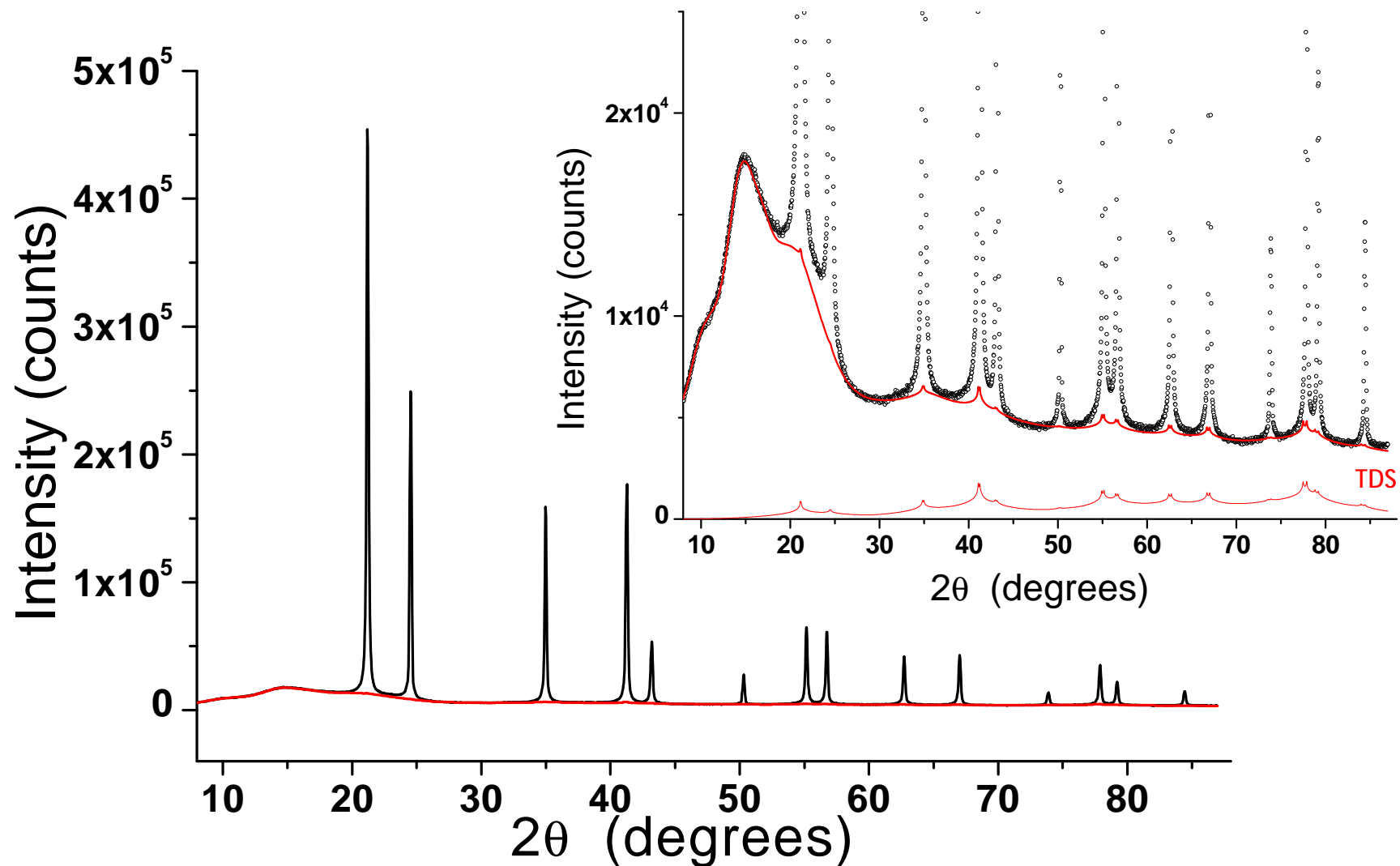
Ø Carefully reproducible / controlled signal from the capillary





DIFFRACTION FROM NANOCRYSTALLINE POWDER

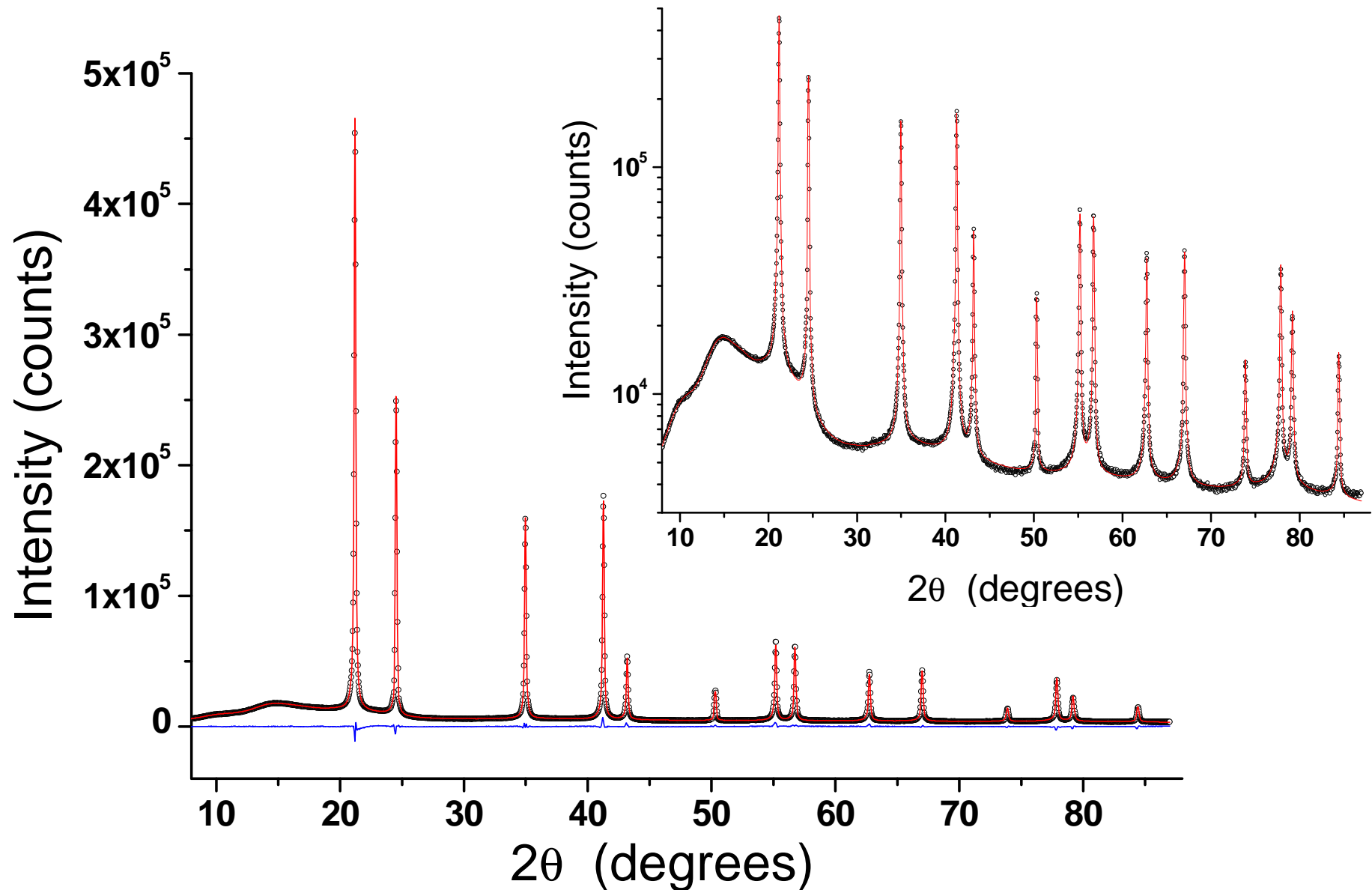
Whole Powder Pattern Modelling (WPPM)





DIFFRACTION FROM NANOCRYSTALLINE *POWDER*

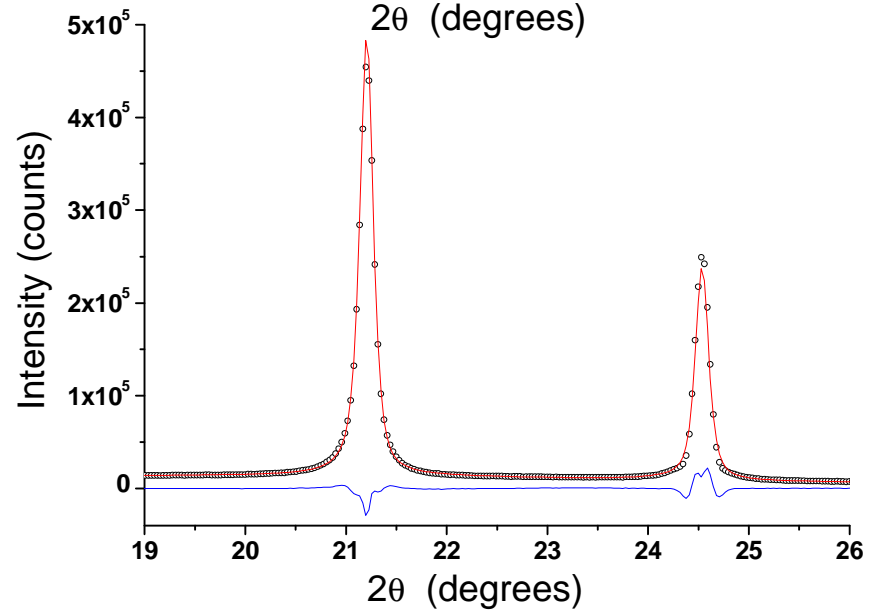
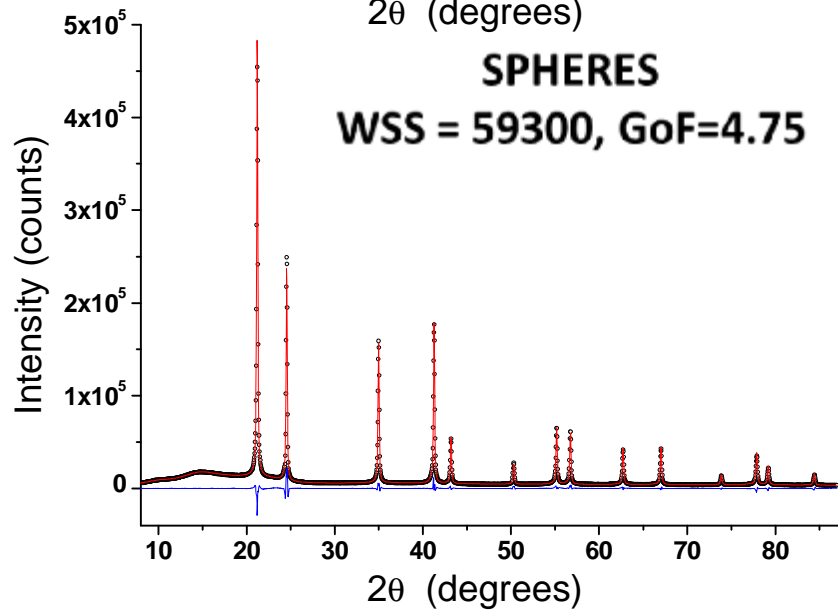
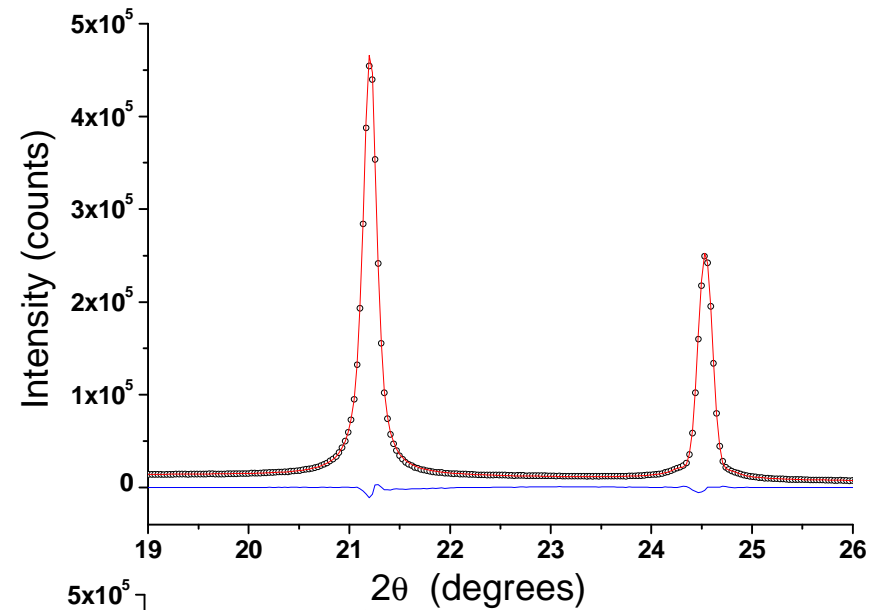
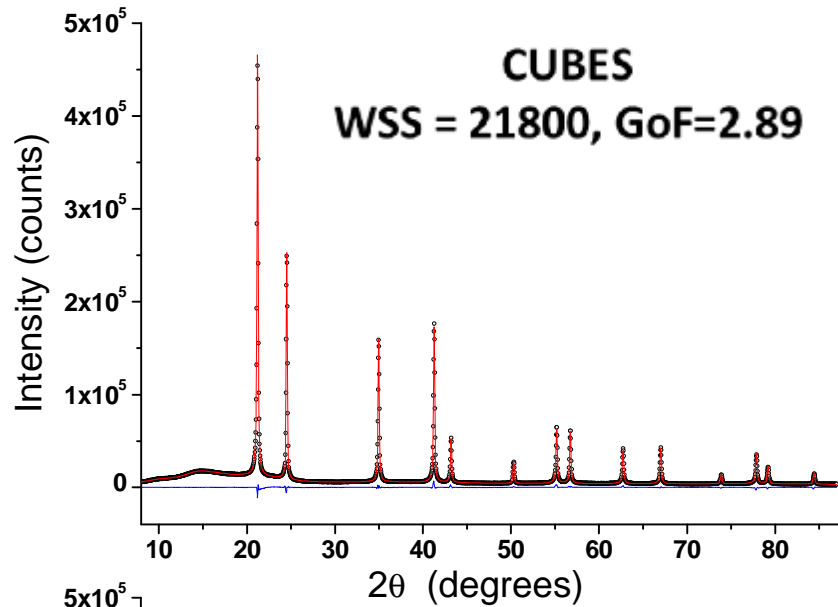
Whole Powder Pattern Modelling (WPPM)





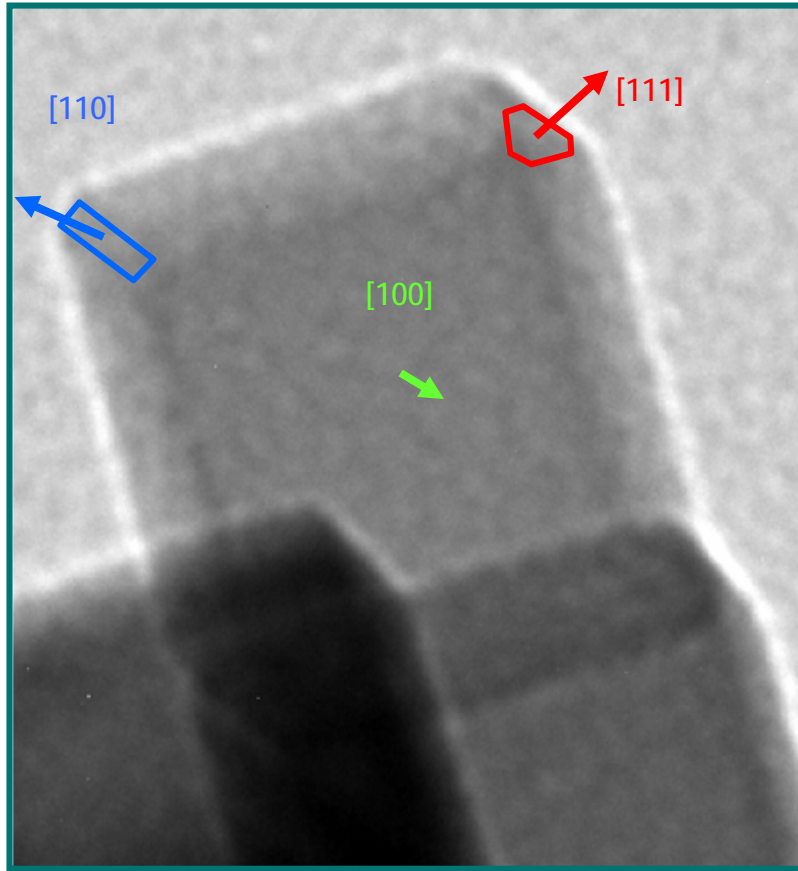
DIFFRACTION FROM NANOCRYSTALLINE *POWDER*

lognormal distribution of cubes vs spheres: shape matters !

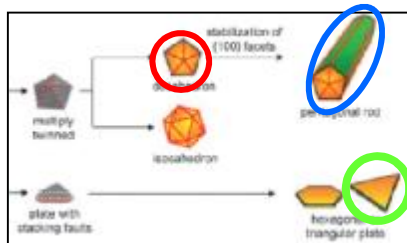
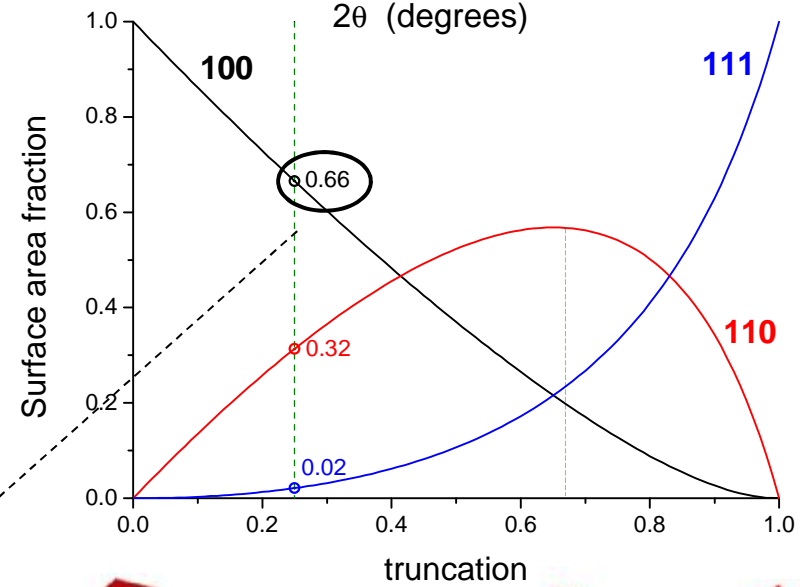
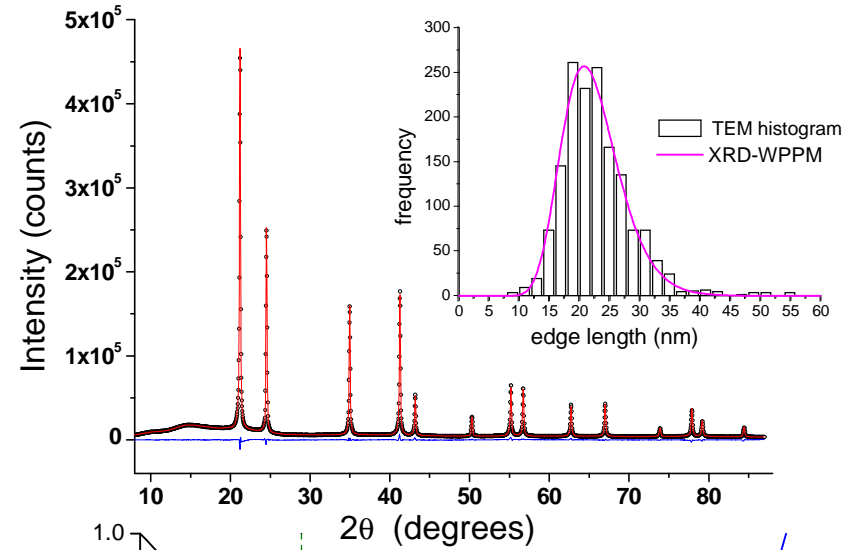




DIFFRACTION FROM NANOCRYSTALLINE *POWDER*



WPPM : truncated cubic Pd nanocrystal



10%



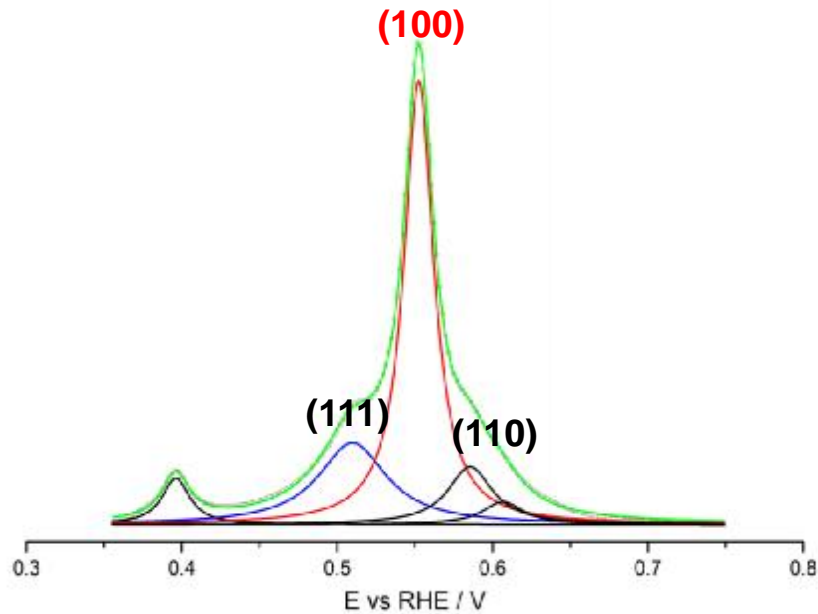
90%



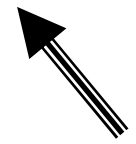
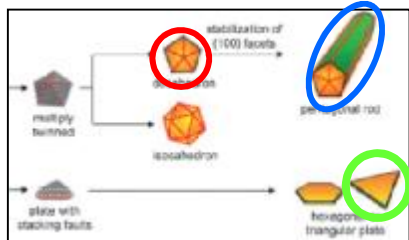


DIFFRACTION & Cu-UPD

Cu Under Potential Deposition (UPD)

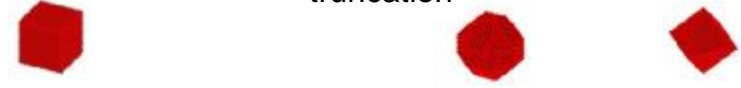
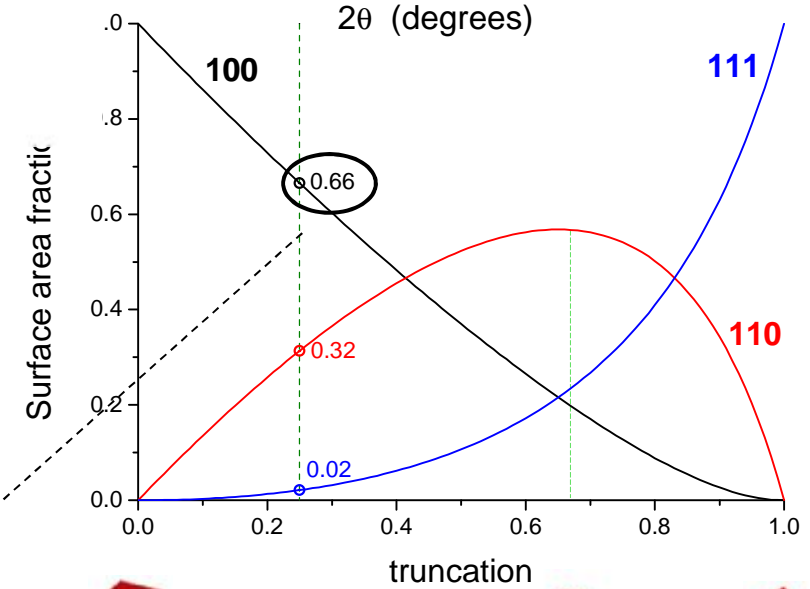
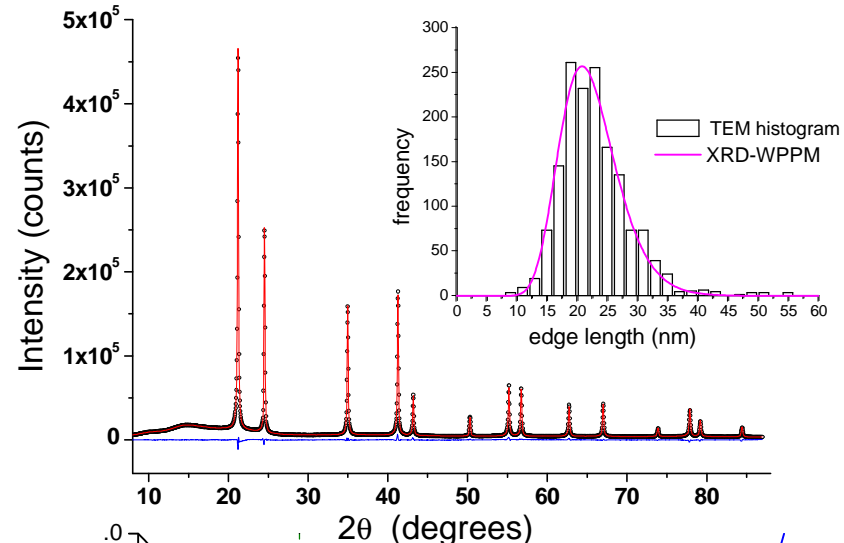


(100) area \approx 55-60 %
 (100) area: 64 %
 (110) area: 28%
 (111) area: 8%



90%

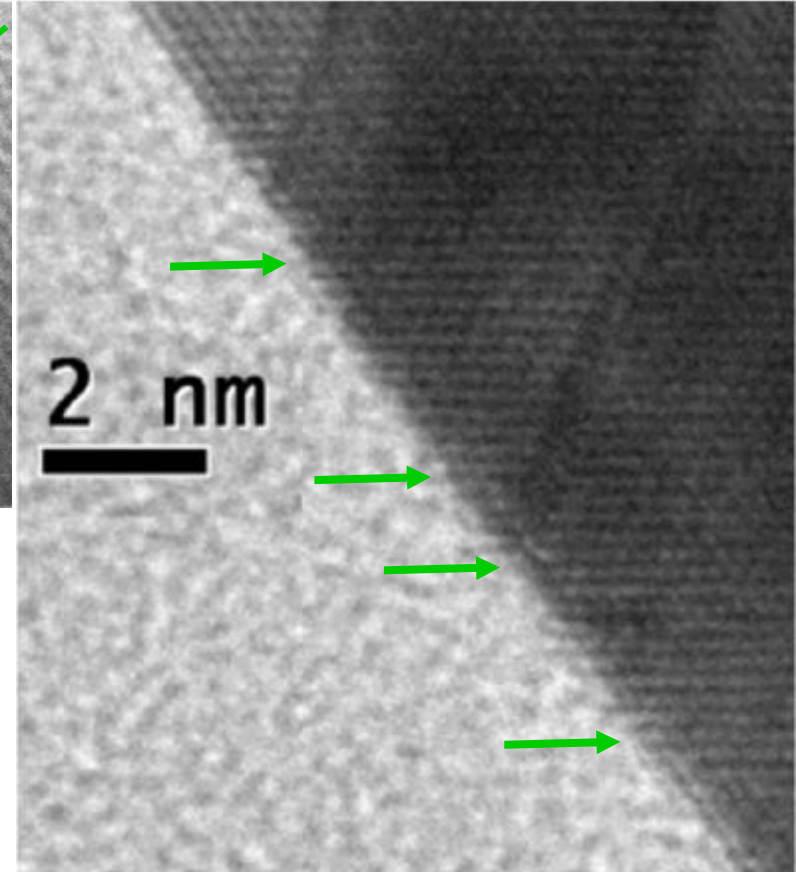
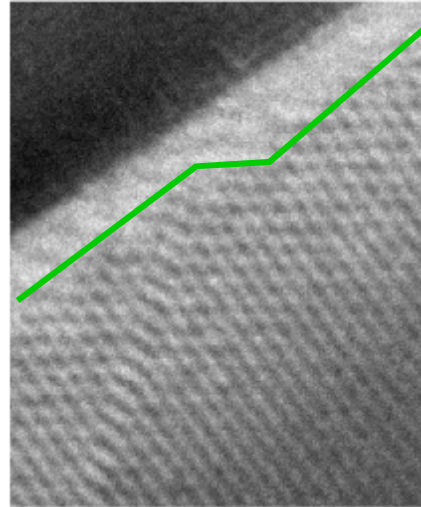
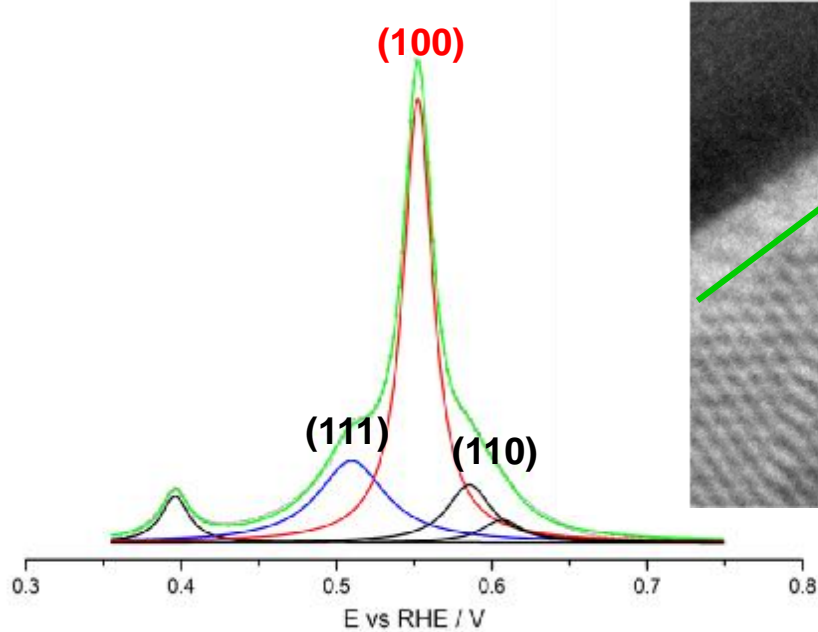
WPPM : truncated cubic Pd nanocrystal





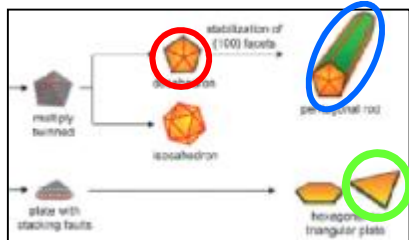
DIFFRACTION, Cu-UPD, HRTEM

Cu Under Potential Deposition (UPD)



(100) area \approx 55-60 %
(100) area: 64 %
(110) area: 28%
(111) area: 8%

»3 steps per
h00 face



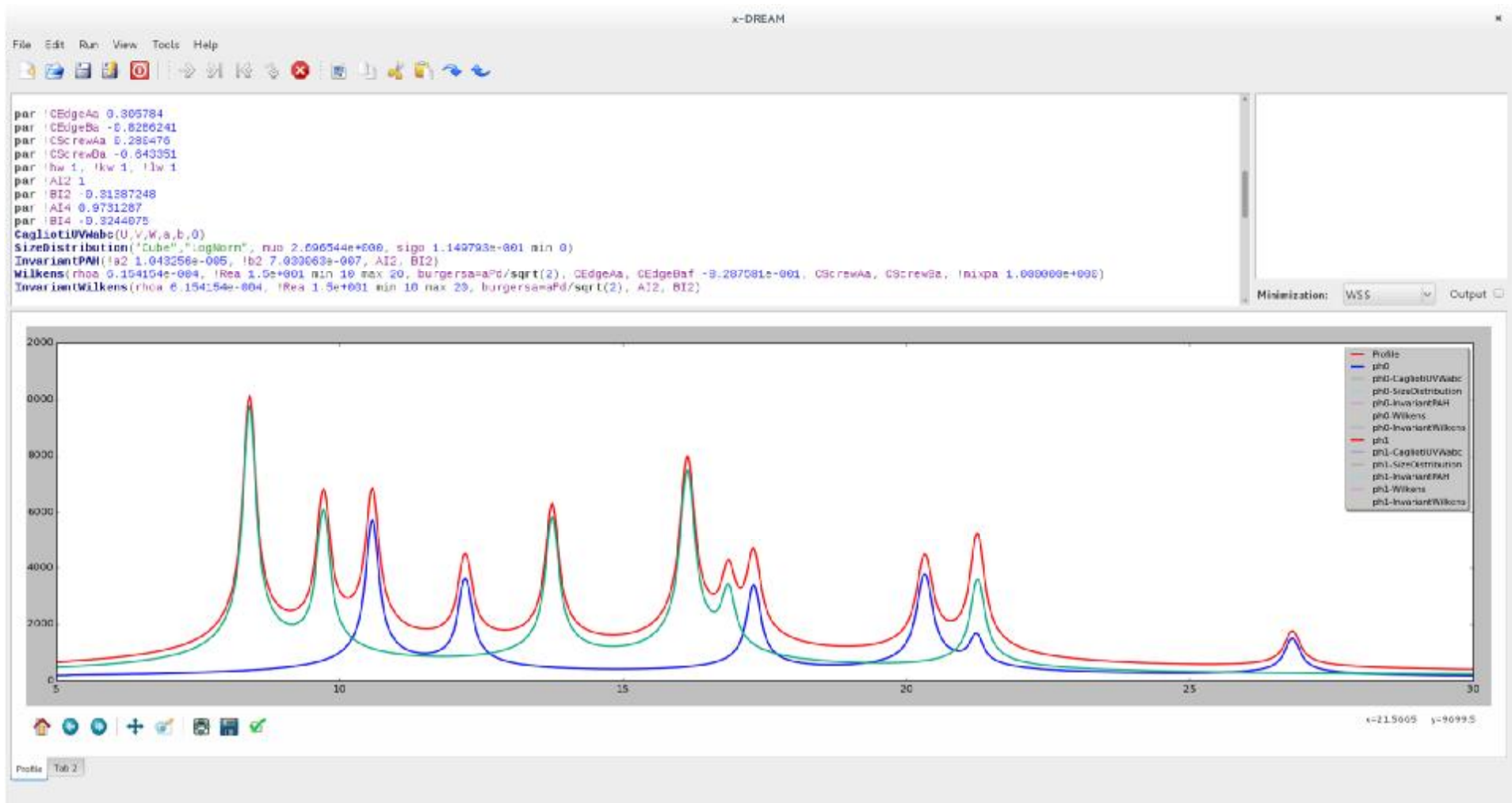
10%



90%



WPPM SOFTWARE: *X-DREAM* EPDI C15 Bari June 2016



- Ø Open source
- Ø Multi -platform, -thread, -programming language based
- Ø Specifically designed to support learning and education