Line broadening analysis

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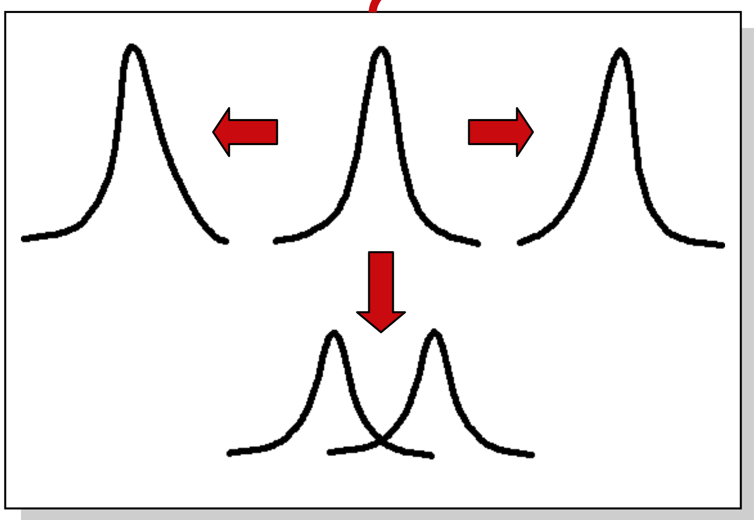
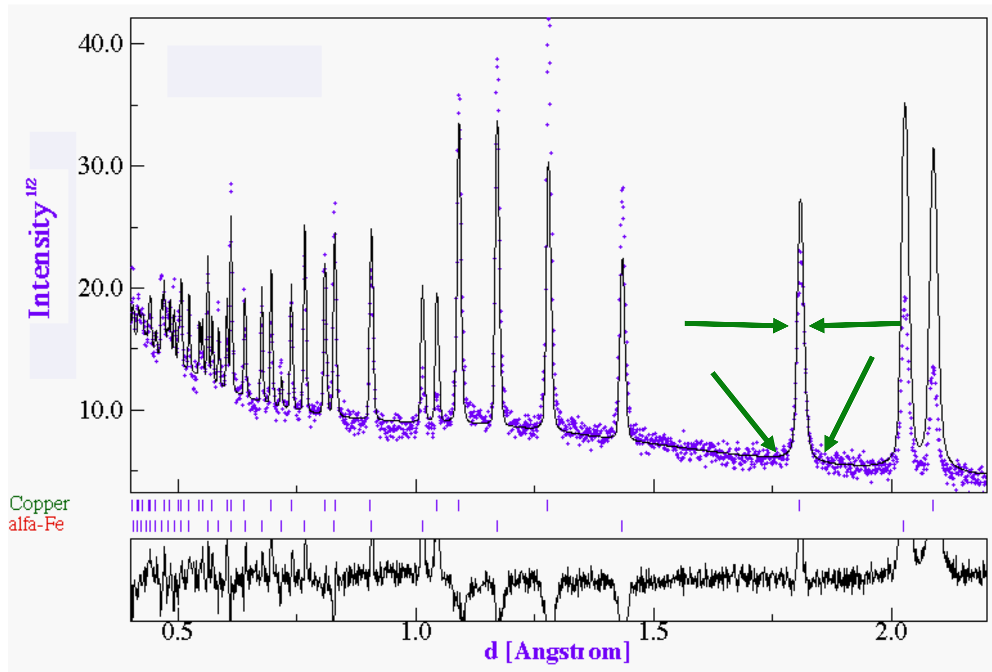
Informations: microstructure

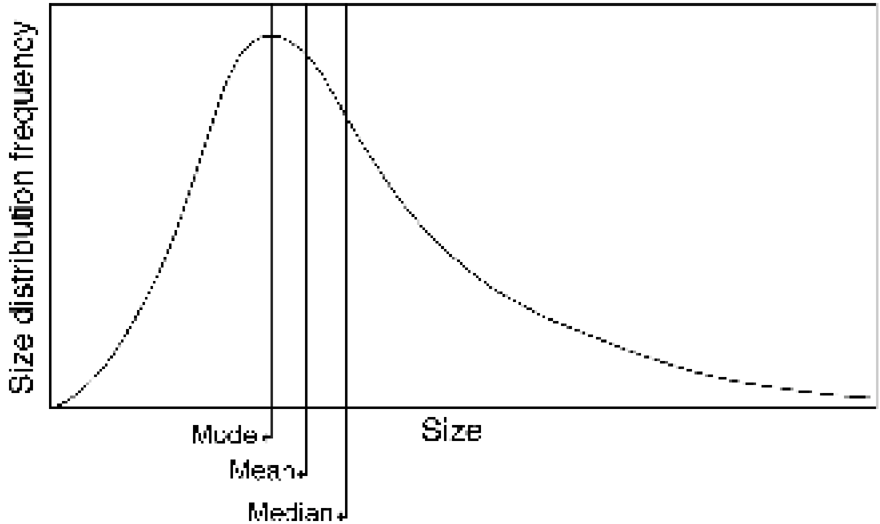
- Crystallite sizes, anisotropic, distribution
- Microstrain (III kind), distribution, dislocation or point defects density
- Antiphase domains (intermetallics…)
- Stacking and deformation faults probability, intrinsic, extrinsic





Crystallites distribution

Name	Definition
Mean length	$\langle M \rangle = \frac{\sum_{i=1}^{N} n_i d_i}{\sum_{i=1}^{N} n_i}$
Length weighted or area-length	$\langle D \rangle = \frac{\sum_{i=1}^{N} n_i d_i^2}{\sum_{i=1}^{N} n_i d_i}$
Area weighted or volume-area	$\langle D_a \rangle = \frac{\sum_{i=1}^{N} n_i d_i^3}{\sum_{i=1}^{N} n_i d_i^2}$
Volume-weighted	$\langle D_V \rangle = \frac{\sum_{i=1}^{N} n_i d_i^4}{\sum_{i=1}^{N} n_i d_i^3}$



Line broadening methods

- **Are based on profile analysis:**
  - **Crystallites and microstrain have a different broadening behavior in 2theta**
- **Several methods available:**
  - **Scherrer equation (1918):**

$$\langle D \rangle_v = \frac{K\lambda}{\beta_S(2\theta)\ \cos\theta}$$

  - **Williamson-Hall plot**
  - **Warren-Averbach or Fourier analysis**
  - **......**
- **Instrumental broadening must be subtracted**
- **Two reflections are needed to separate crystallite and microstrain broadening**
- **More reflections for anisotropic broadening**
- **Planar defects analysis was developed by Warren (see book)**

The Warren-Averbach analysis

Warren treatment for a 00l peak:

$$S(2\theta) = \int S_S(2\theta - z) S_I(z)\, dz$$

(Stokes treatment: $A = A_S A_I$)

Fourier coefficients:

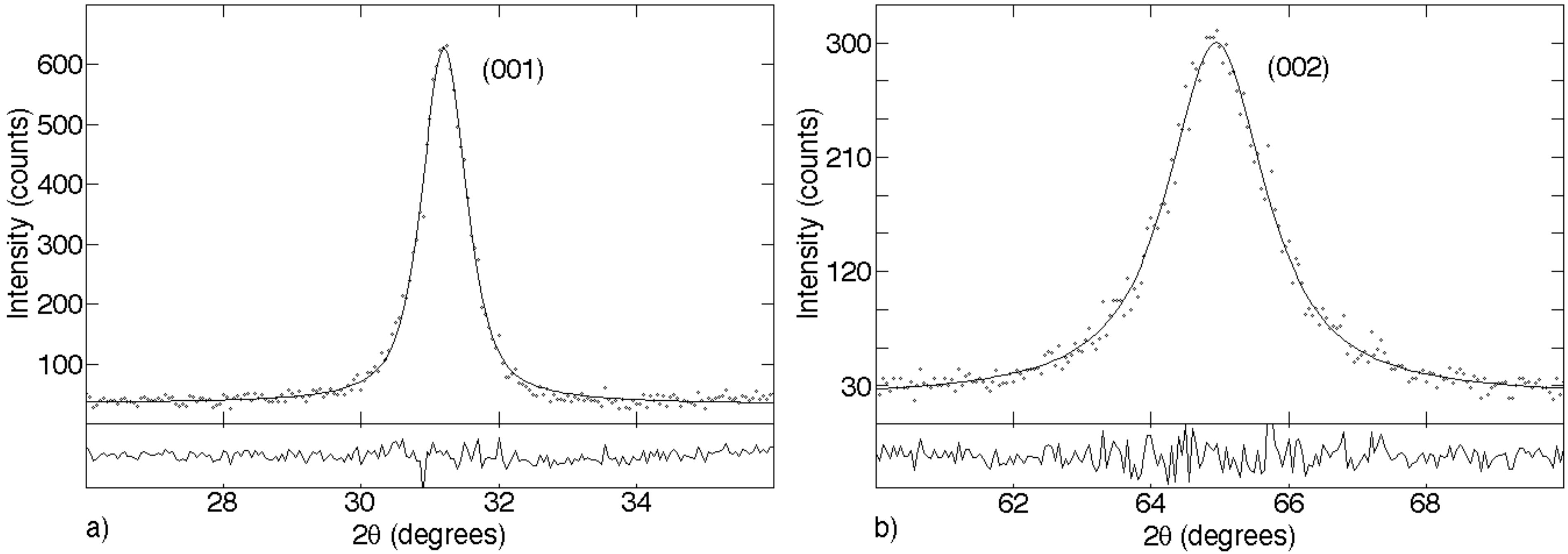
$$A_n = A_n^S A_n^D = \frac{N_n}{N_3} \langle \cos 2\pi l Z_n \rangle$$

$$A_n^S = \frac{N_n}{N_3} = \frac{1}{N_3} \sum_{i=|n|}^{\text{inf}} (i - |n|)\, p(i)$$

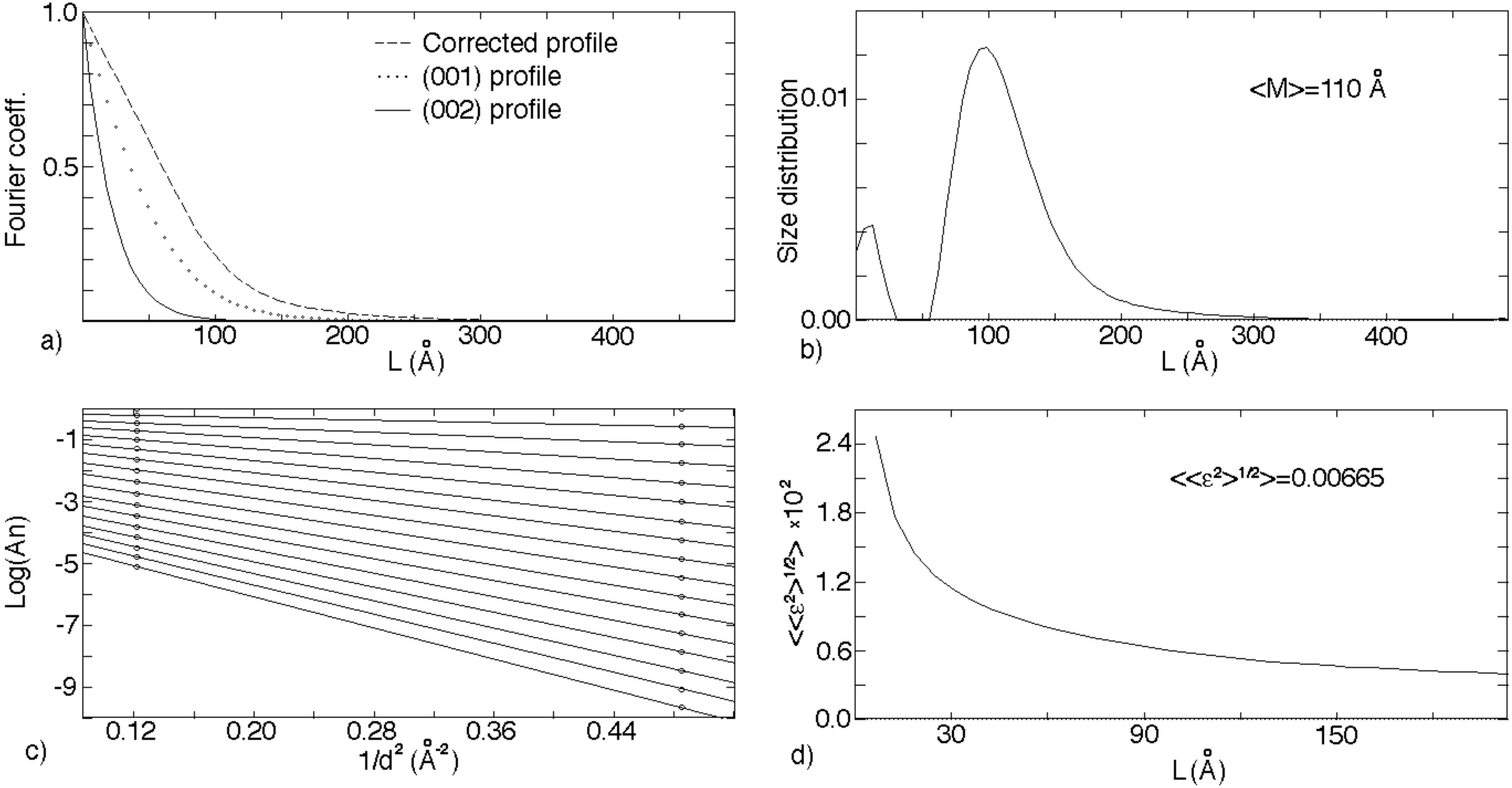
$$\left(\frac{dA_n^S}{dn} \right)_{n \to 0} = -\frac{1}{N_3}$$

Get the profiles for Fourier transform

We need two peaks of different order, same hkl direction

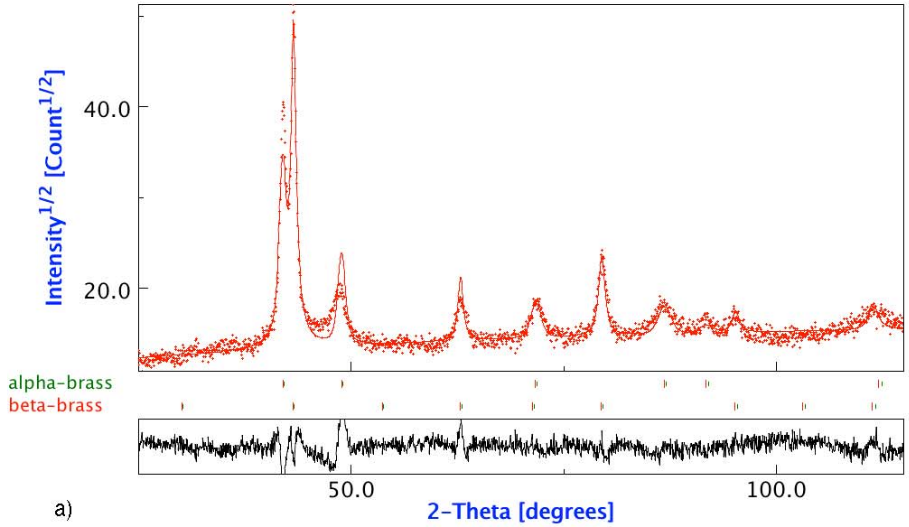


W-A continue.....



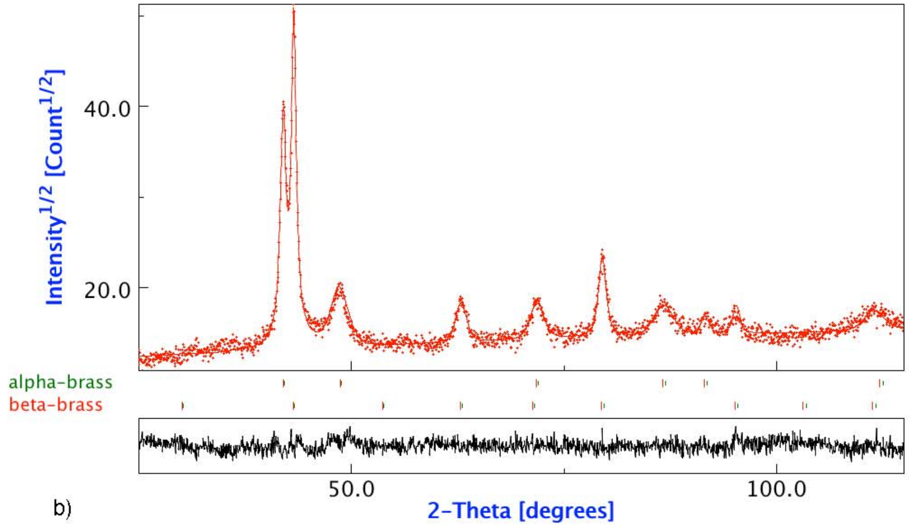
Corrected profile
(001) profile
(002) profile
Fourier coeff.
1.0
0.5
100
200
300
400
L (Å)
a)
Size distribution
<M>=110 Å
0.01
0.00
b)
Log(An)
-1
-3
-5
-7
-9
0.12
0.20
0.28
0.36
0.44
1/d² (Å⁻²)
c)
<<ε²>^1/2> x10²
<<ε²>^1/2>=0.00665
2.4
1.8
1.2
0.6
0.0
30
90
150
d)

Planar faults



a)

No faults assumed

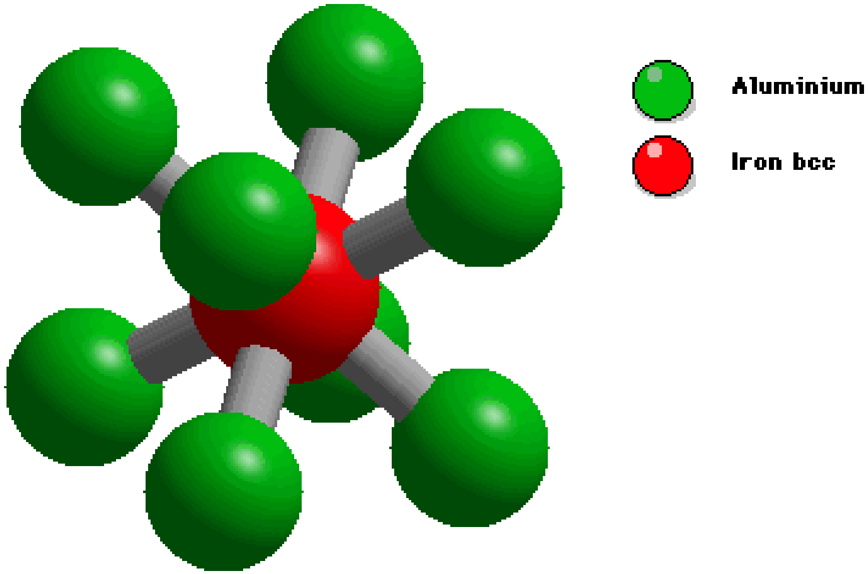


b)

Stacking and deformation faults

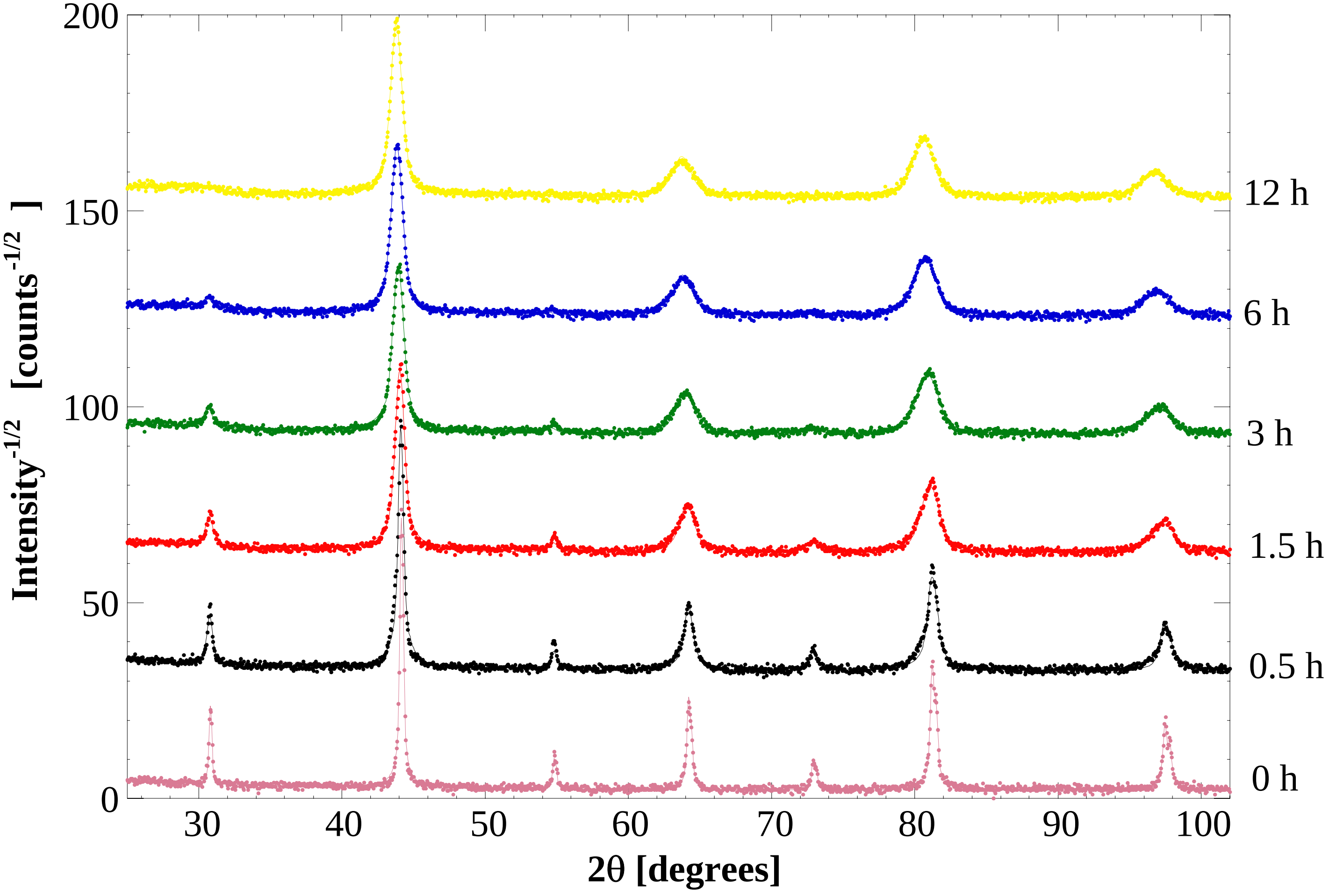
Order-disorder transition in intermetallic

- **Applications:**
  - High temperature structural material
  - Oxidation resistance
  - Blade material for Gas turbine
- **Main problem:**
  - Ductility (forming and shaping)
  - Brittle at low temperature
- **Disordered phase is more ductile**



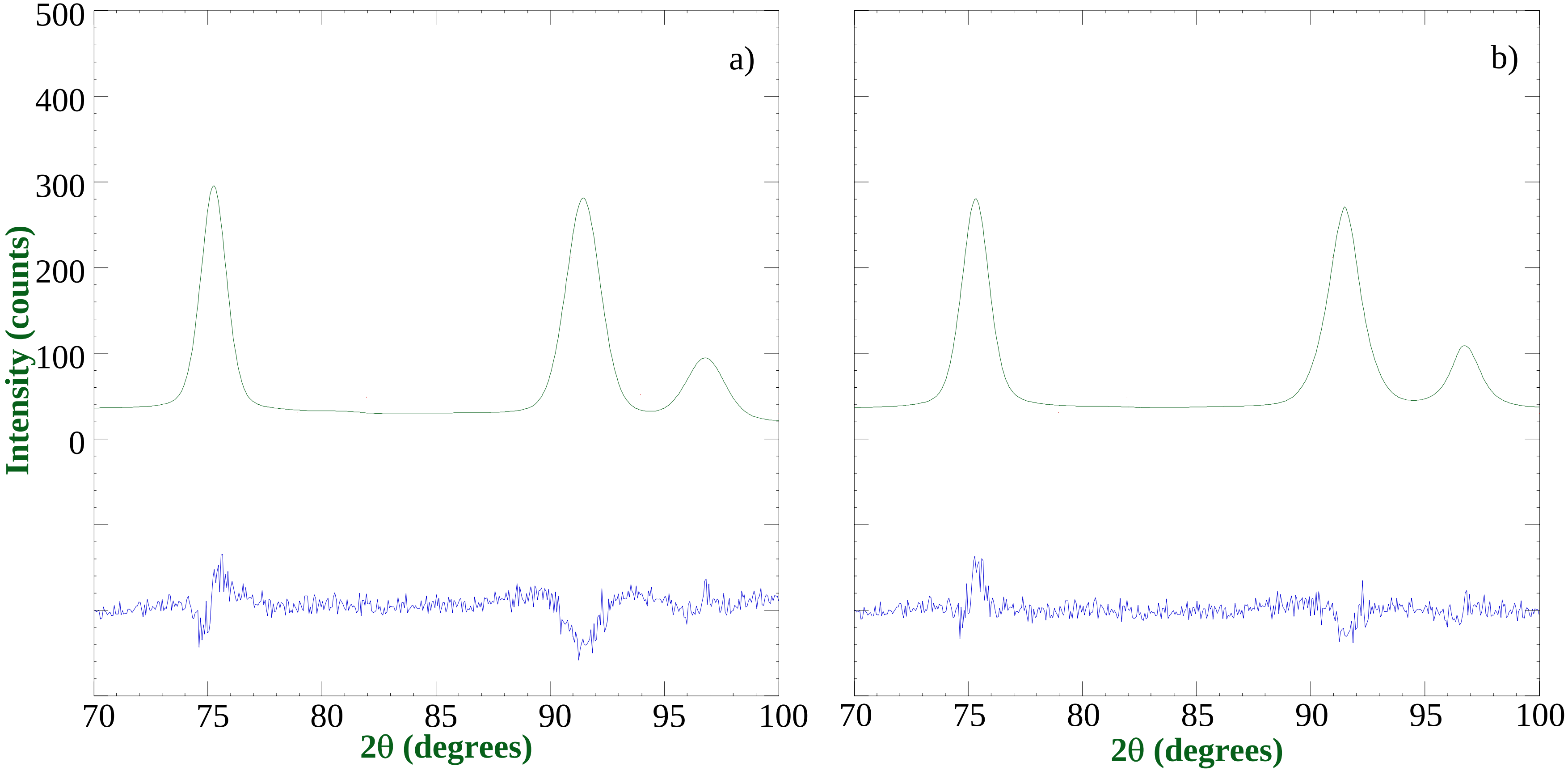
- **Materials:**
  - FeAl, Ni_3Al, NiAl, TiAl...

Disordering FeAl by ball-milling

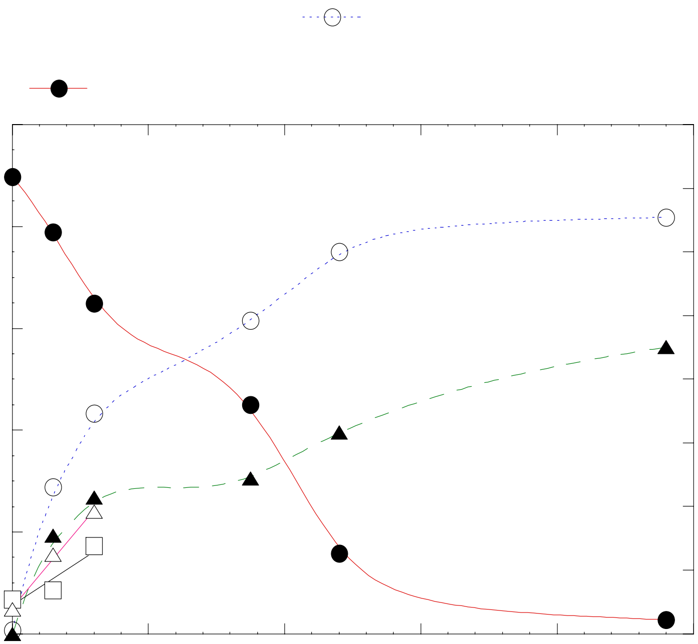


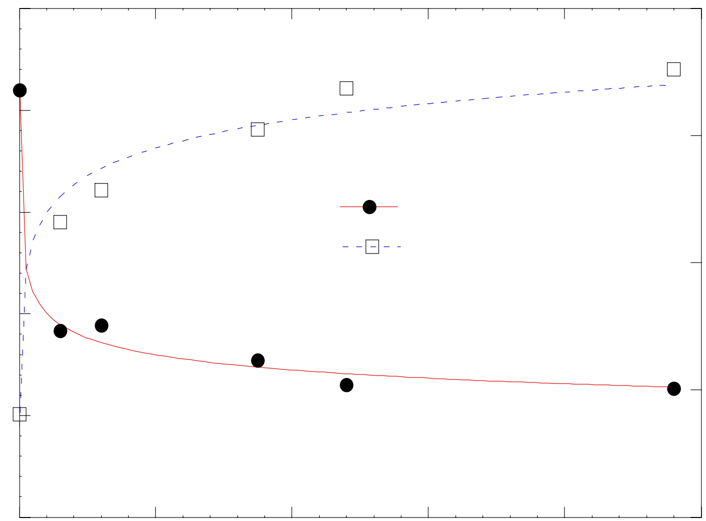
Faults effect

Anisotropic size model **Faulting model (Warren)**



Defect analysis on ball-milled FeAl





FeAl annealing (neutron-XRD meas.)