

Coarsening Dynamics in Elastically Anisotropic Phase-Separating Alloys with XPCS

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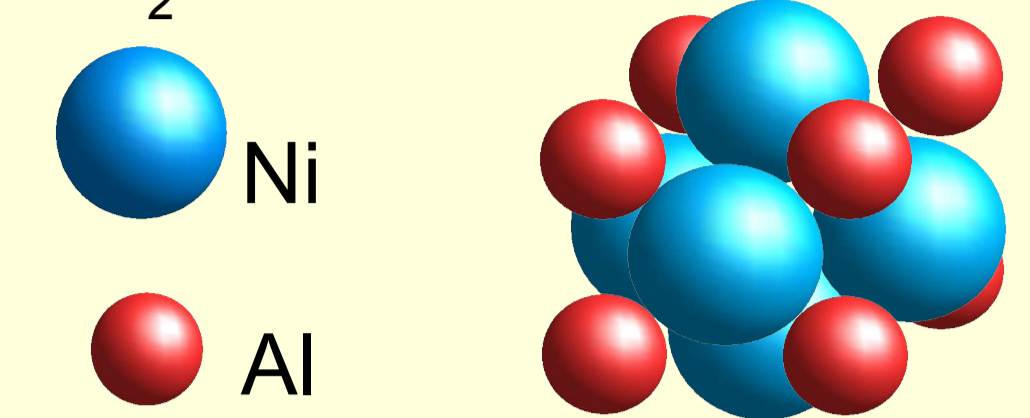
Coarsening in Ni-Al-Mo

In the late stage of phase-separation in alloys coarsening occurs. The main driving force for this process is the interface energy. Additionally, if the lattice constants of the precipitates (a_p) and the matrix (a_m) do not match, elastic interactions play a crucial role. Our aim is to study the dynamical properties of these processes.

Two separating phases:

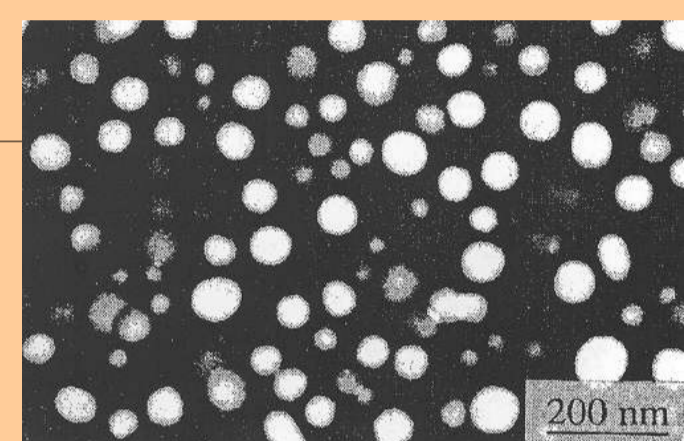
- Ni-rich: disordered fcc (matrix)
 - Ni₃Al: L1₂-ordered (precipitates)
- Misfit (δ) controlled by Mo content

L1₂-structure:



$$\delta = \frac{a_p - a_m}{a_m}$$

Misfit and elastic anisotropy define shape and alignment of the precipitates in the matrix



Misfit $\delta = 0$
shape: spherical
alignment: random
Picture: M. Fähmann et al, Acta metall. mater. 43, 1007 (1995).



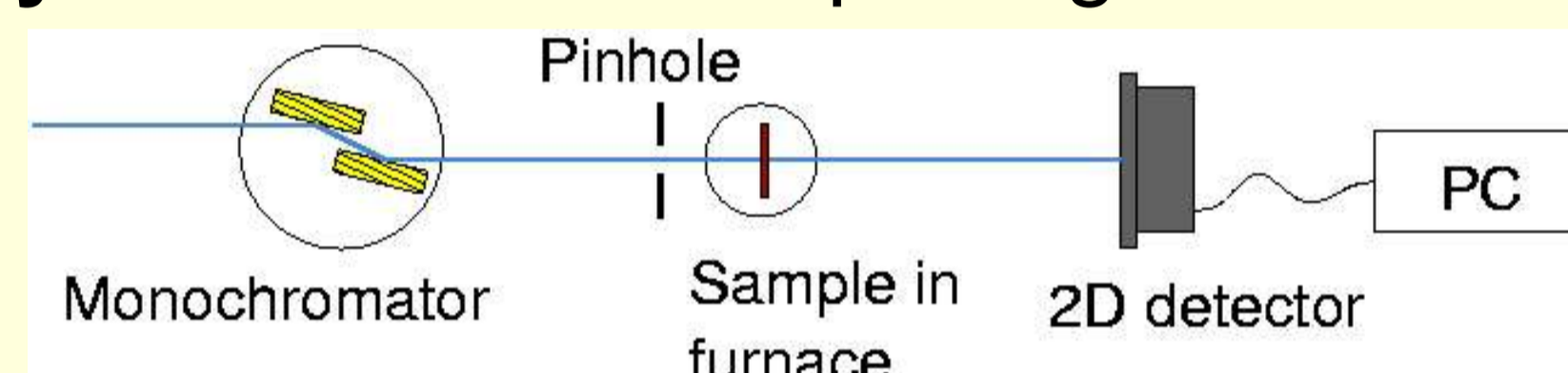
Misfit $|\delta| > 0$
shape: cuboidal or plate-like
alignment: along elastic soft directions $\langle 001 \rangle$
Picture: J.-M. Schneider, B. Schönfeld, B. Demè, and G. Kosterz, J. Appl. Cryst. 33, 465 (2000).

XPCS

X-ray Photon Correlation Spectroscopy

Scattering of **coherent radiation** at a disordered sample causes a highly modulated diffraction pattern, a so-called **speckle pattern**. This interference pattern changes with the motion of the scattering centres in the coherently illuminated material. By analysing the **temporal correlations of intensity fluctuations** information about the **dynamics** in the sample is gained.

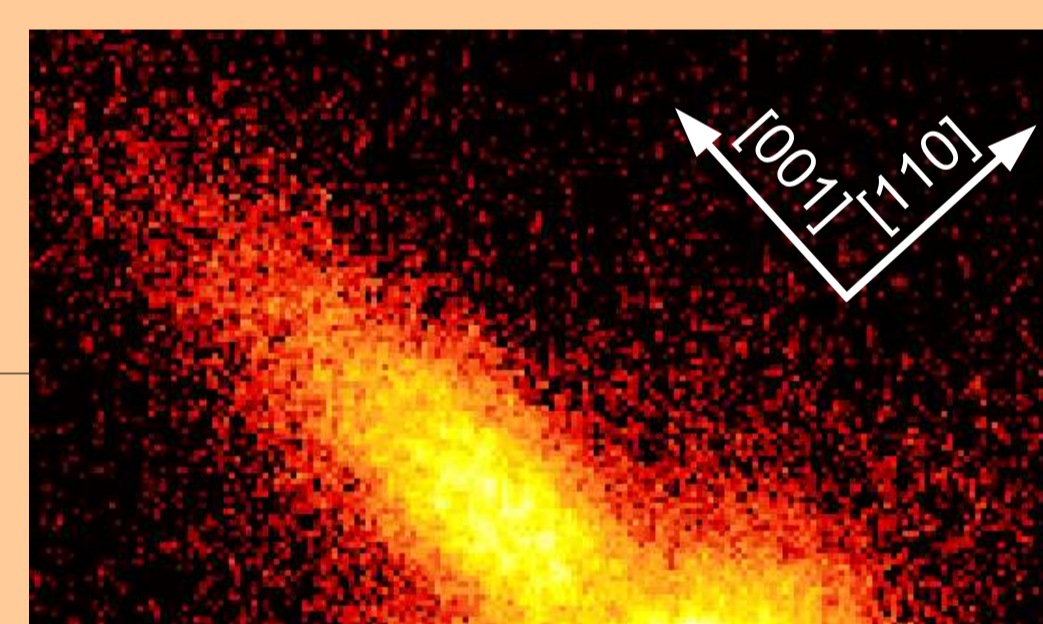
Measurements in small-angle X-ray scattering geometry.



SAXS-pattern with speckles

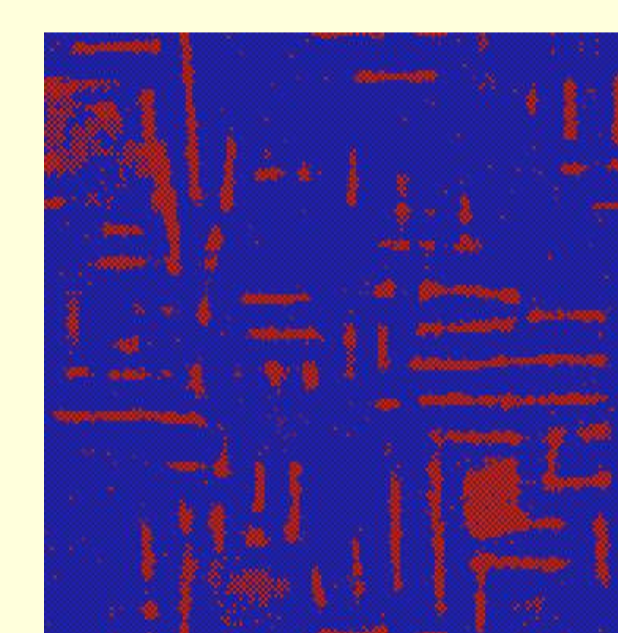
$\delta=0$

$\delta=+0.65\%$



MCS

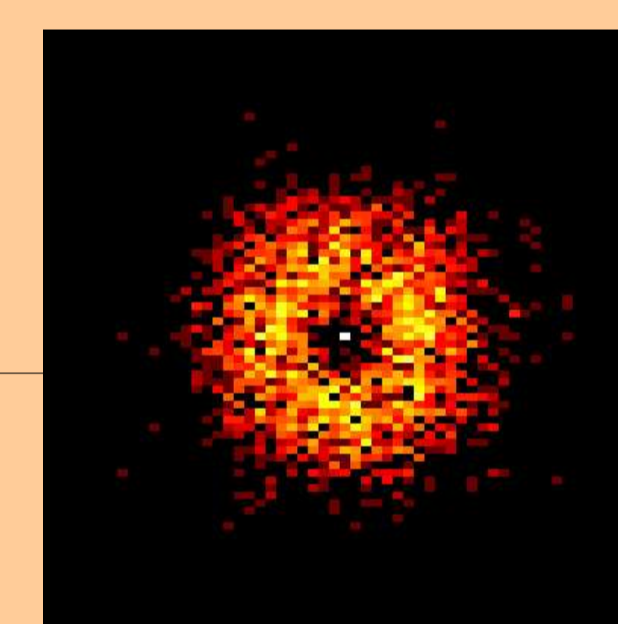
Monte Carlo Simulations



top view on a (001) cut, positive lattice misfit, 2000MCS

The model:

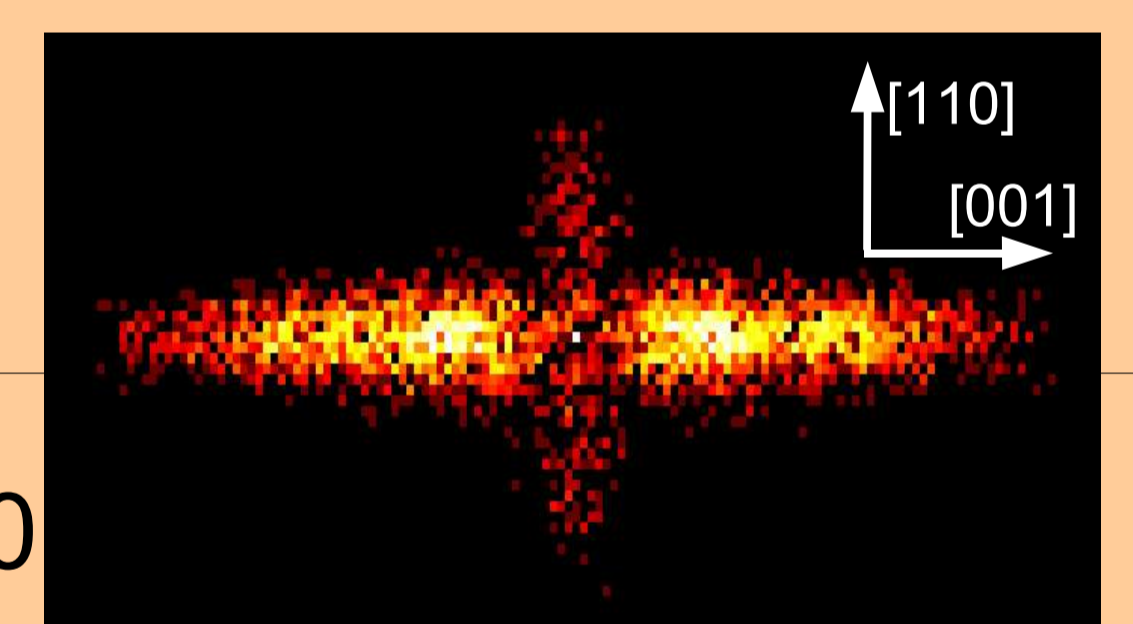
- two types of atoms in an fcc lattice
- atoms connected with springs
- elastic and chemical interaction
- 96x96x96 lattice
- periodic boundary conditions



Simulated pattern

$\delta=0$

$\delta>0$

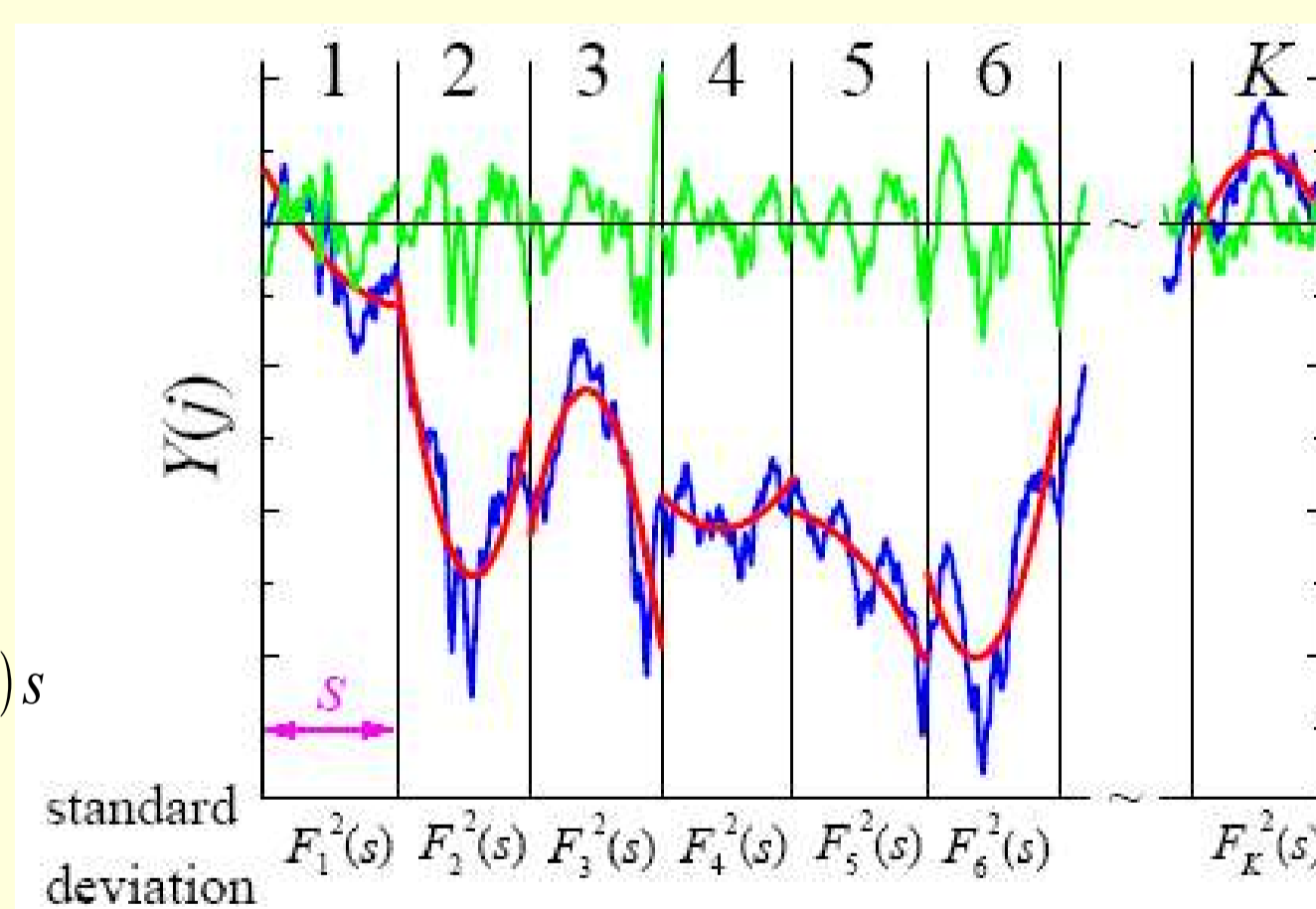


DFA

Detrended Fluctuation Analysis

DFA procedure:

- Recording of time-dependent intensity fluctuations
- Calculate the "profile" of the fluctuation $Y(j) = \sum_{i=1}^j I_i$
- Split the record into K segments
- Perform a **polynomial fit** in each segment $P_n(j)$
- Determine the **variance** $F_n^2(s) = \langle (Y(j) - P_n(j))^2 \rangle_{j=(n-1)s}^{ns}$
- Average over all segments $F(s) = \left[\frac{1}{K} \sum_{n=1}^K F_n^2(s) \right]^{1/2}$

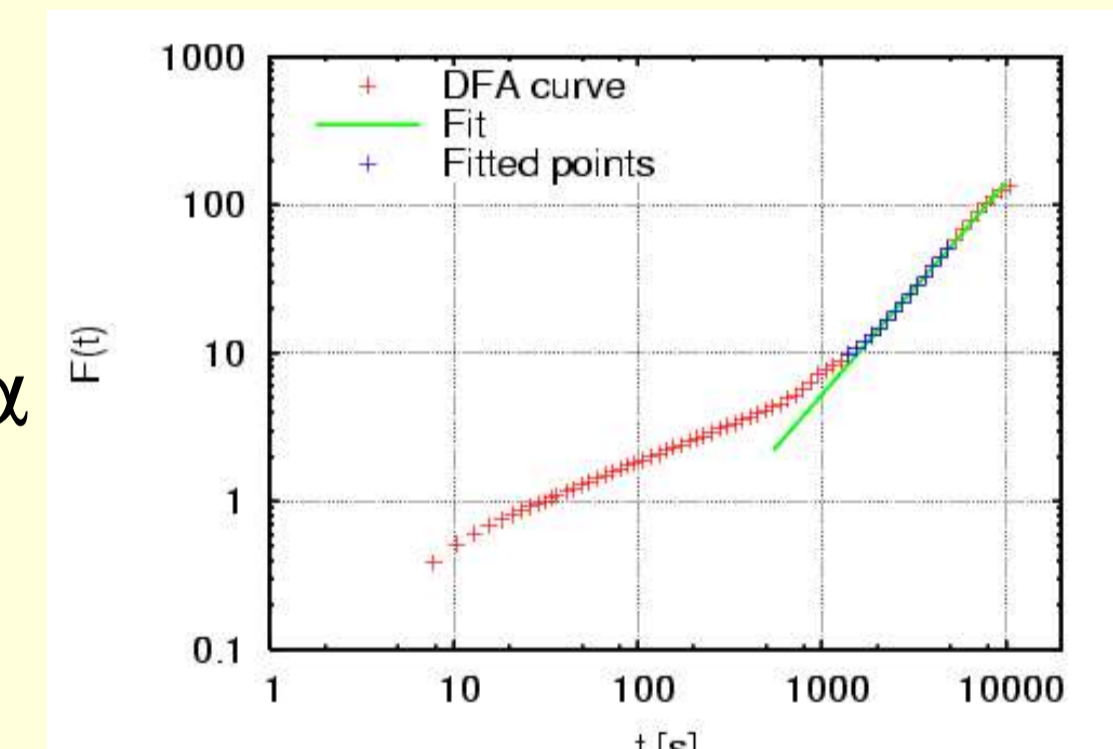


- Fit fluctuation exponent α

$$F(s) \propto t^\alpha$$

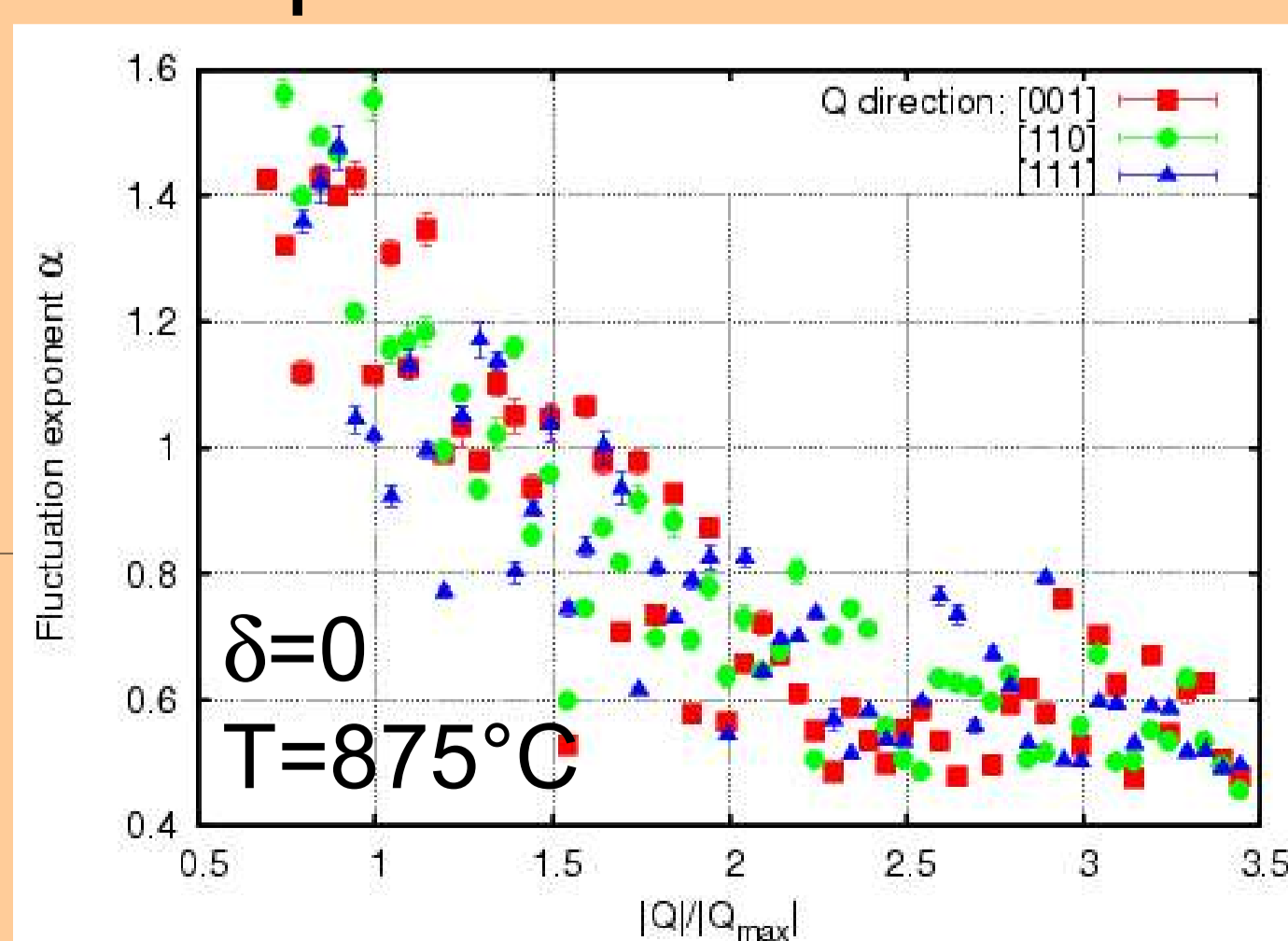
- Random uncorrelated fluctuations: $\alpha=0.5$

- Random walk fluctuations: $\alpha=1.5$

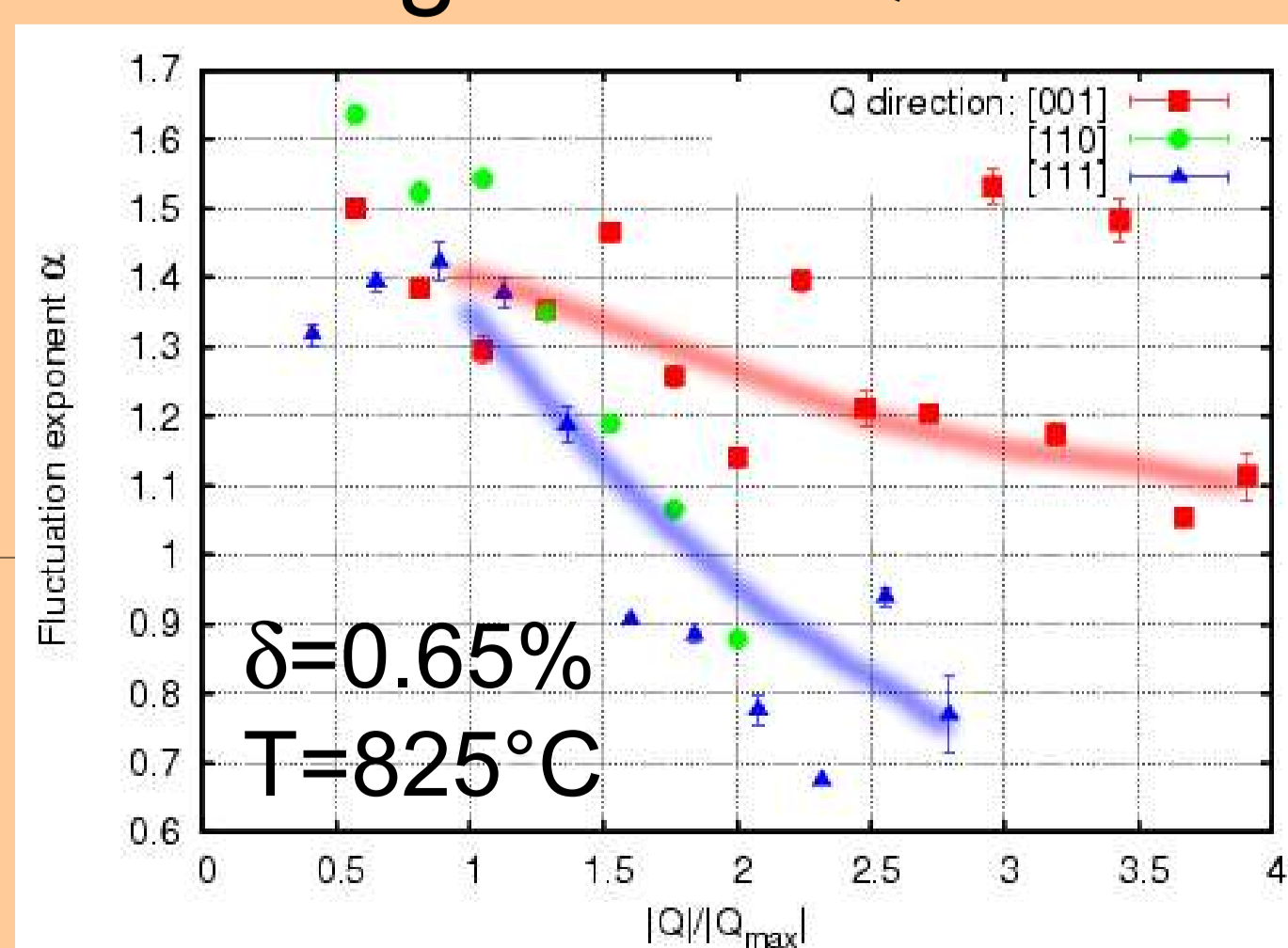


Typical DFA curve with uncorrelated noise on shorter time scales and a fit to the correlated part.

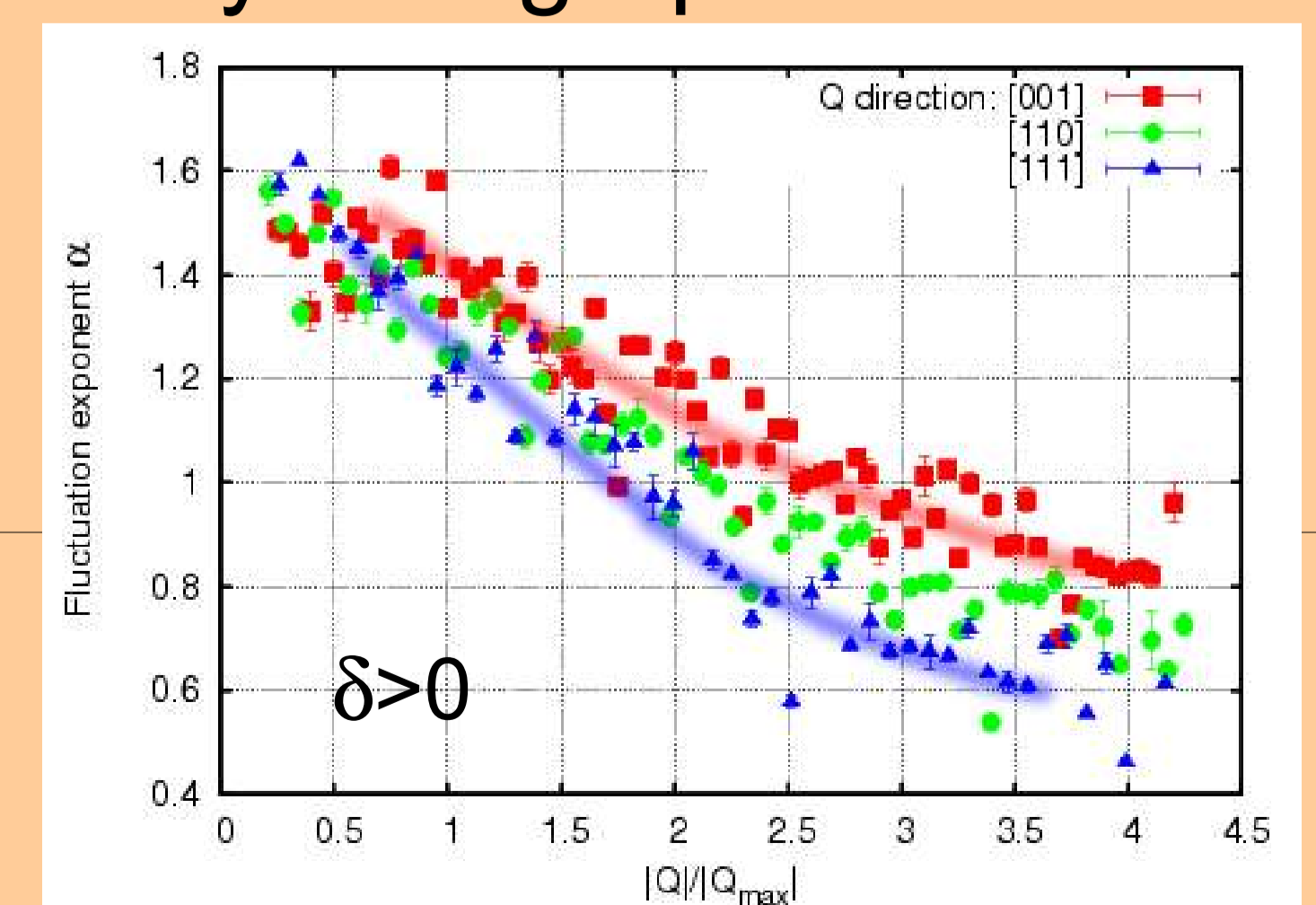
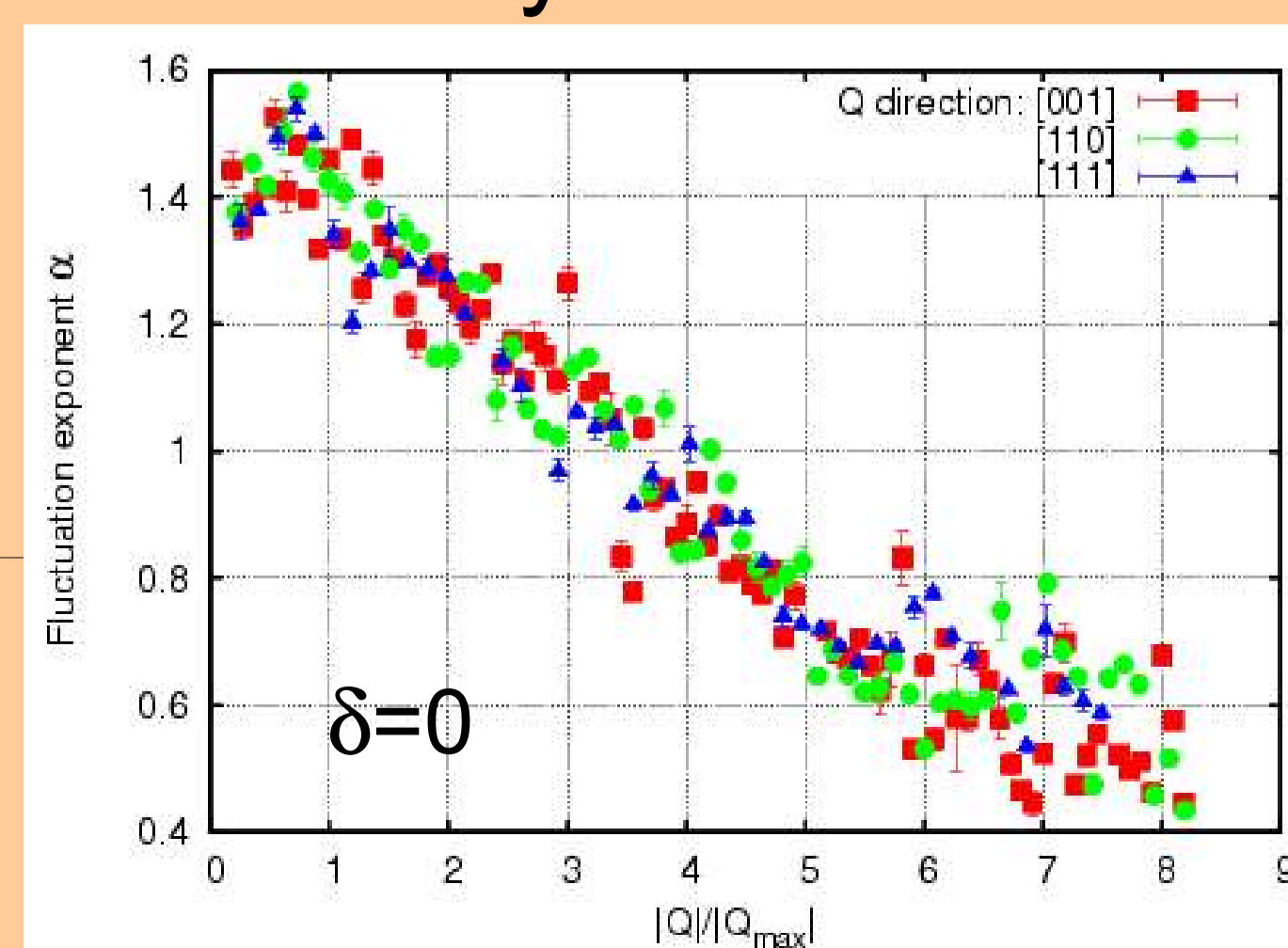
The dependence of α on the scattering vector Q indicates different dynamics in different crystallographic directions.



Results from XPCS experiments



Results from Monte Carlo Simulations



Preliminary conclusion: Precipitate atoms are locked along the elastic soft directions.