

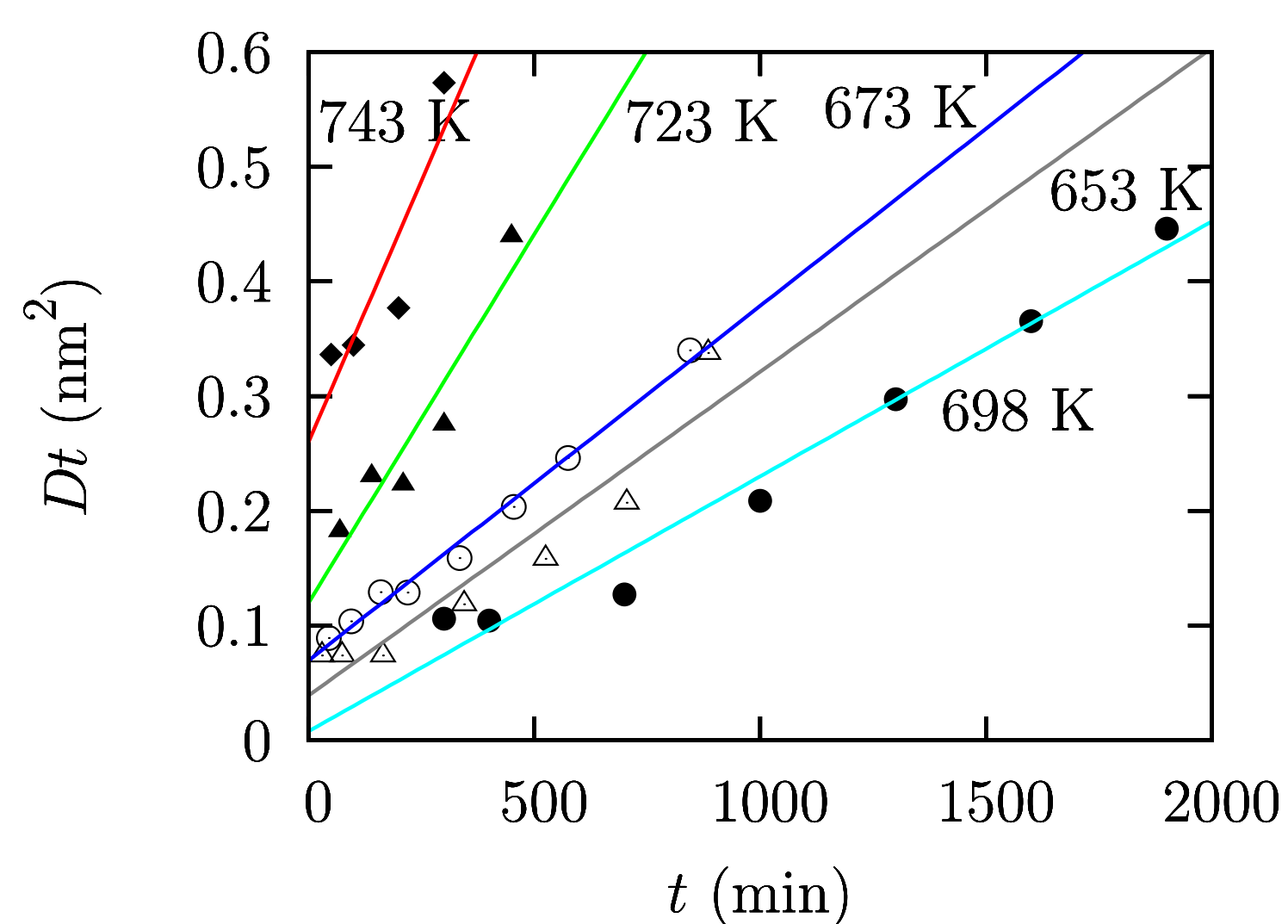
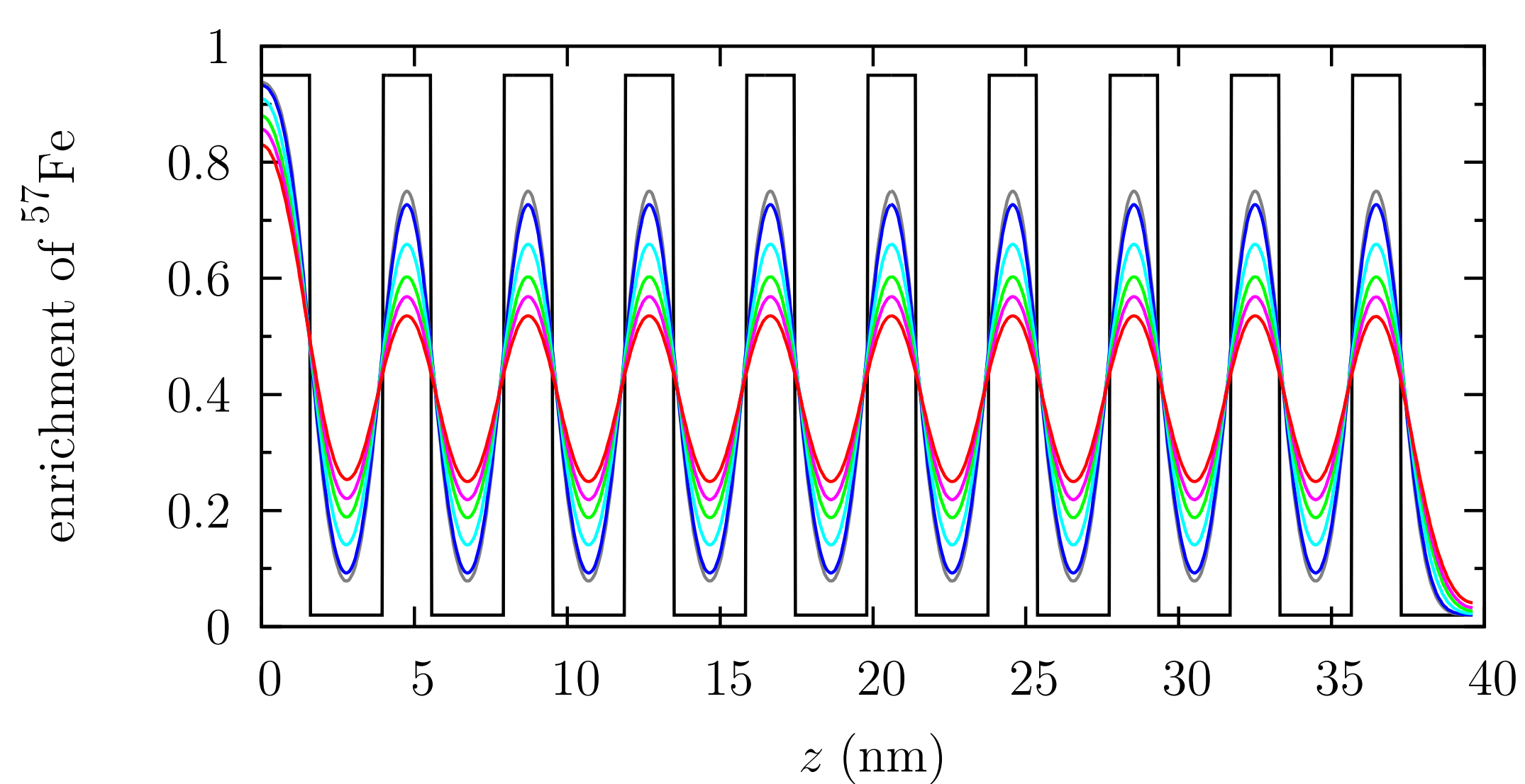
## INTRODUCTION

Nuclear Resonant Scattering (NRS) on isotopically varying but chemically homogeneous multilayers allows us to study diffusion coefficients down to  $10^{-25} \text{ m}^2\text{s}^{-1}$  with high resolution of the diffusion length [1].

Up to now only the kinematical theory has been applied to evaluate the experimental data, however this approach was criticized in a recent paper [2], which led to further analysis, taking dynamical effects into account.

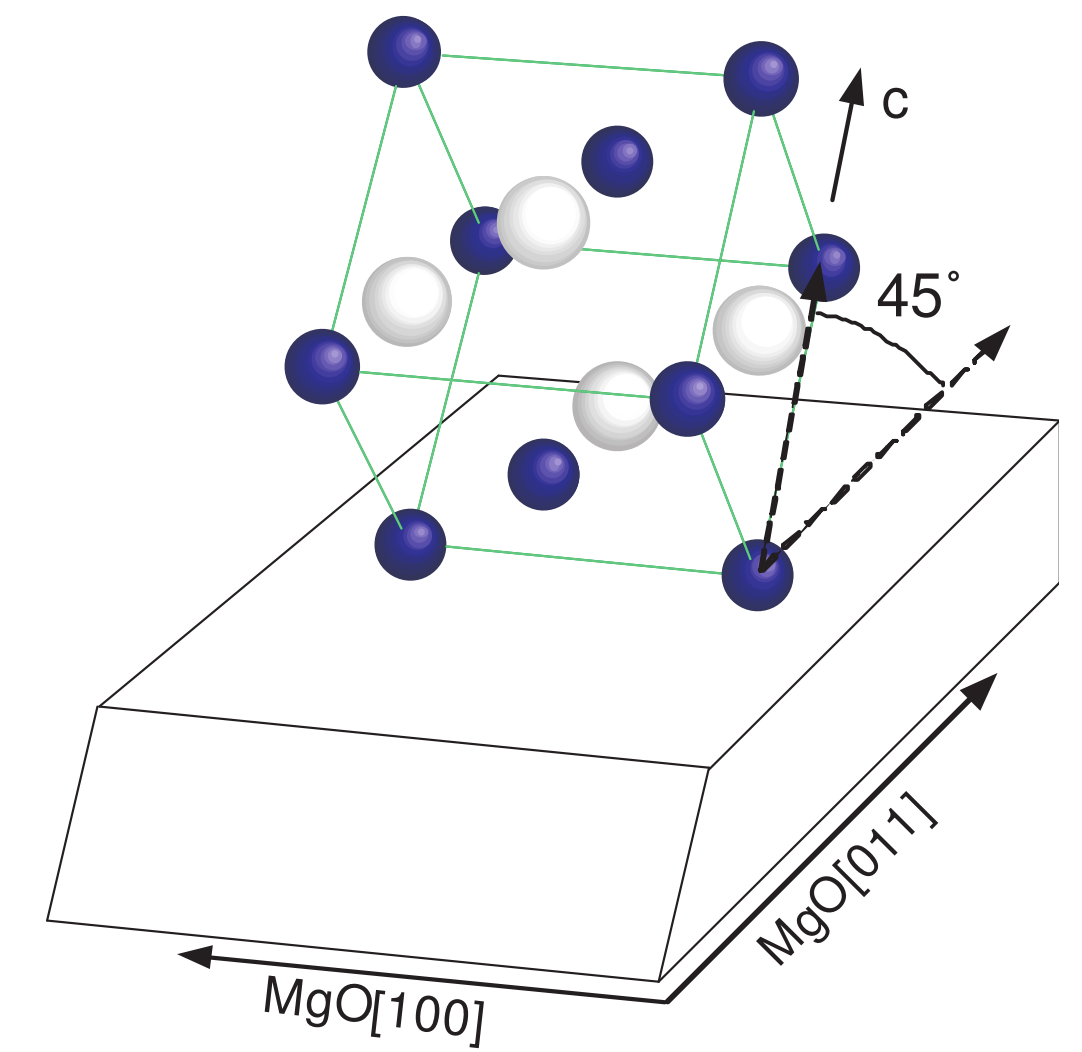
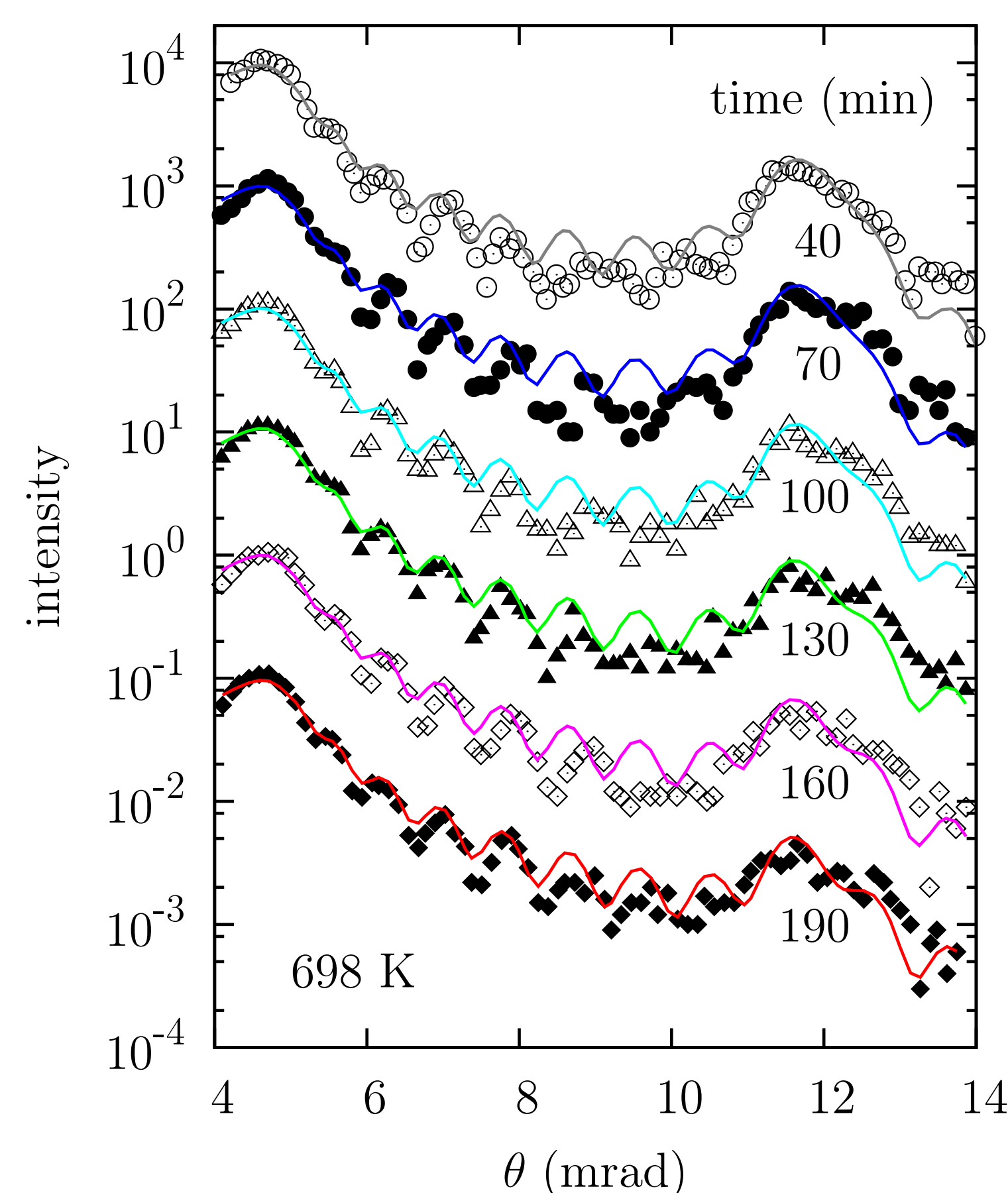
## SIMULATION & FIT

The diffusion equation is solved by convolution of the fundamental solution with the initial value function  $g(x)$ . The boundary conditions are incorporated by reflection of this function at the origin.



The scattering intensity in grazing incidence of the discretized diffuse isotopic system is currently calculated by the program package CONUSS [3]. The resulting fits are shown in the upper right figure for a sample annealed at 698 K measured at ESRF, Grenoble.

This procedure was done for 5 temperatures, several time steps each, leading to the figure on the left. The time scales of the 3 spectra with filled data points were multiplied by 10 for better visibility.



## THEORY

The standard approach via kinematical approximation leads to

$$\ln \left( \frac{I_m(t)}{I_m(0)} \right) = \frac{8\pi^2 m^2}{d^2} Dt \quad (1)$$

for the intensities of the  $m$ -th order Bragg peaks with the structure period  $d$ .

For the dynamical theory we first have to solve the diffusion equation for constant diffusion coefficient  $D$

$$\partial_t c(t, x) = D \partial_x^2 c(t, x) \quad (2)$$

with the fundamental solution

$$c(t, x) = (4\pi Dt)^{-1/2} \exp(-x^2/4Dt) \quad (3)$$

and von Neumann boundary conditions

$$\begin{cases} c(0, x) = g(x) \\ \partial_x c(t, a) = \partial_x c(t, b) = 0 \end{cases} \quad (4)$$

Nuclear Resonant Scattering (NRS) on homogeneous layer with propagation matrix  $\mathbf{F}$

$$\partial_z \mathbf{A}(z) = i\mathbf{F}\mathbf{A}(z) \quad (5)$$

NRS on diffuse isotopic multilayer discretized into  $N$  homogeneous layers  $j$  with thicknesses  $d_j$

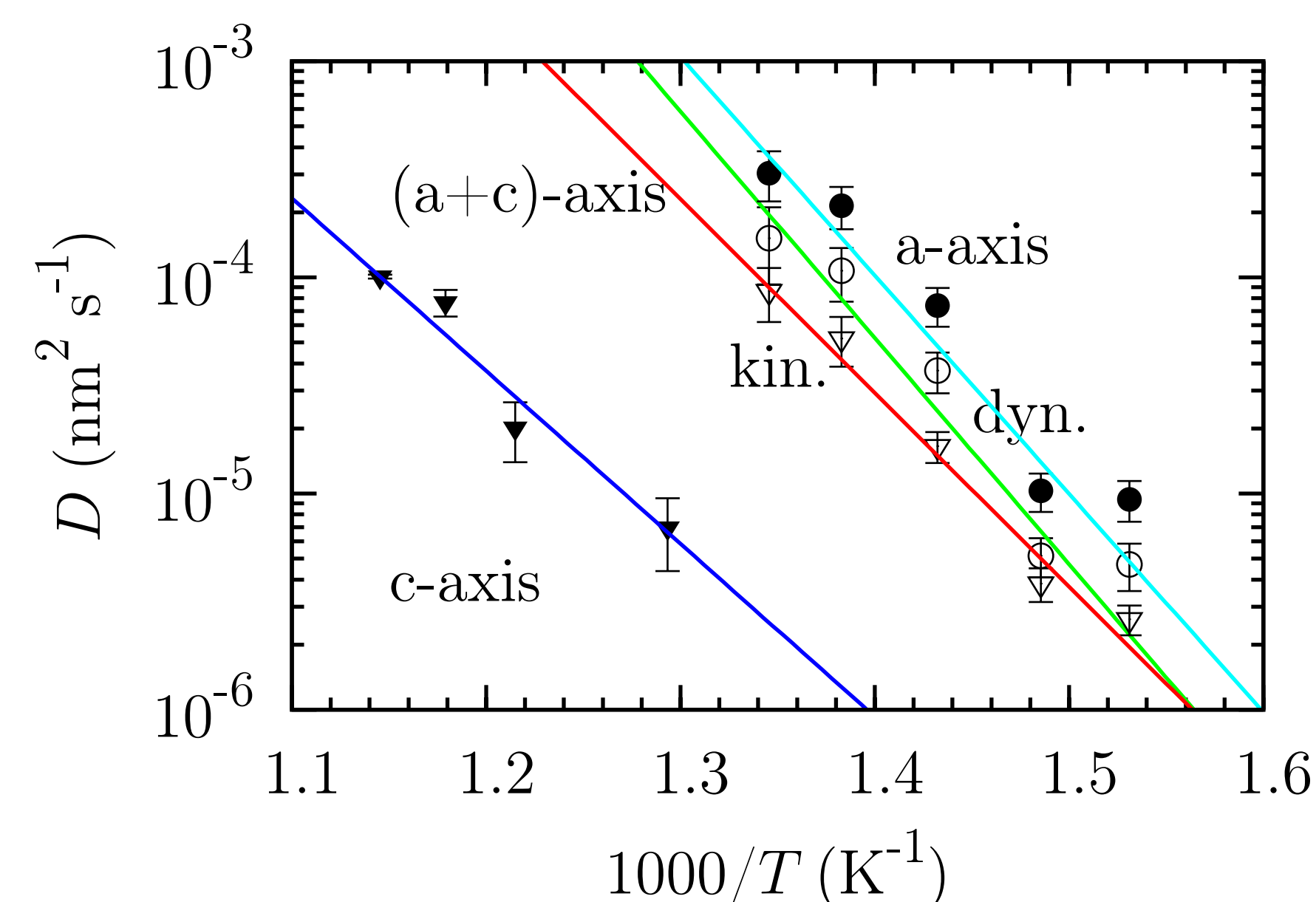
$$\mathbf{A}(z) = e^{i\mathbf{F}_N d_N} \dots e^{i\mathbf{F}_1 d_1} \mathbf{A}(0) \quad (6)$$

## DIFFUSION COEFFICIENT

Taking into account the number of nearest neighbors and projections on the axis of measurement, one can find the simple geometrical relation

$$D_a = 2D_{110} - D_c \quad (7)$$

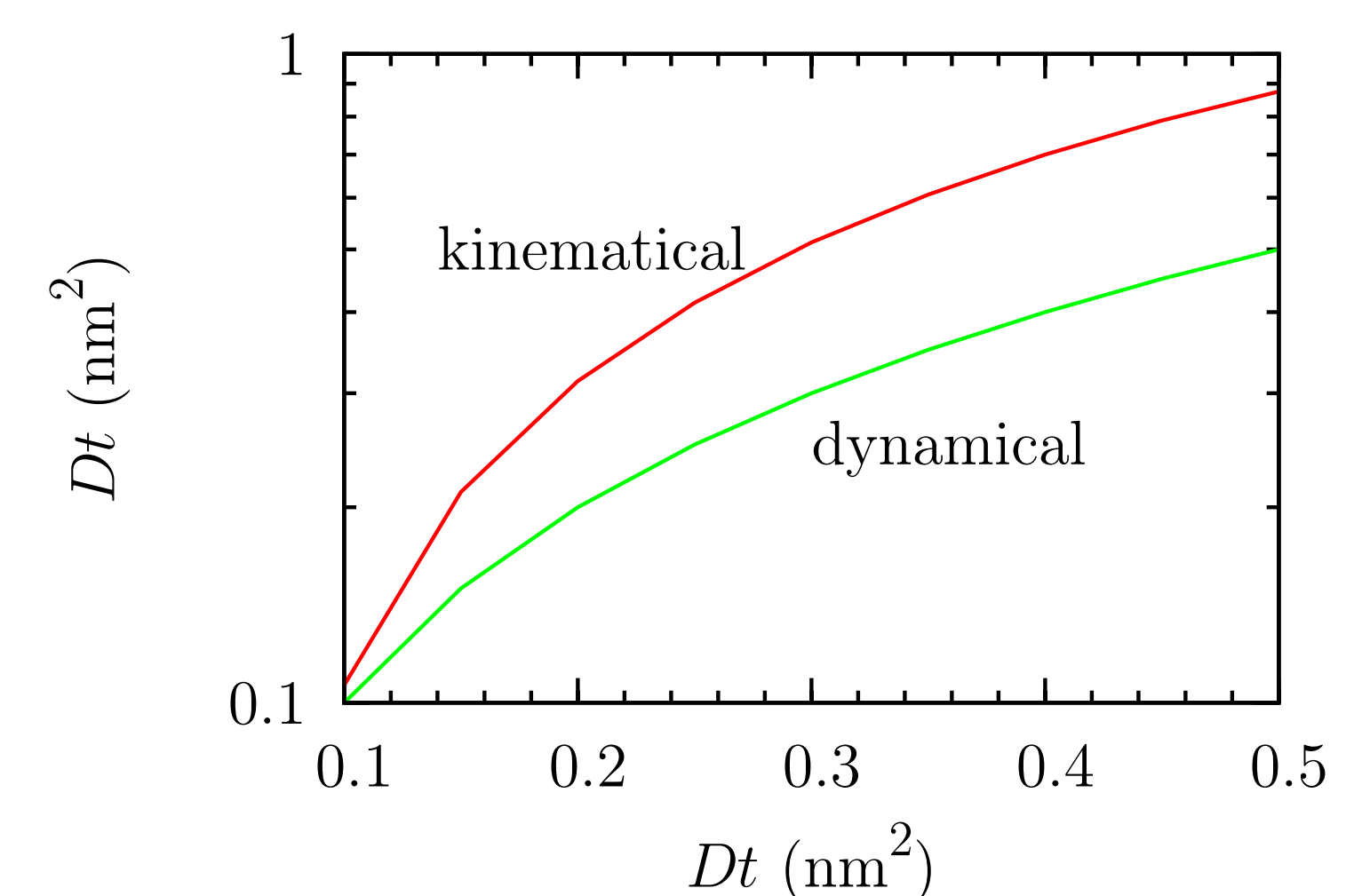
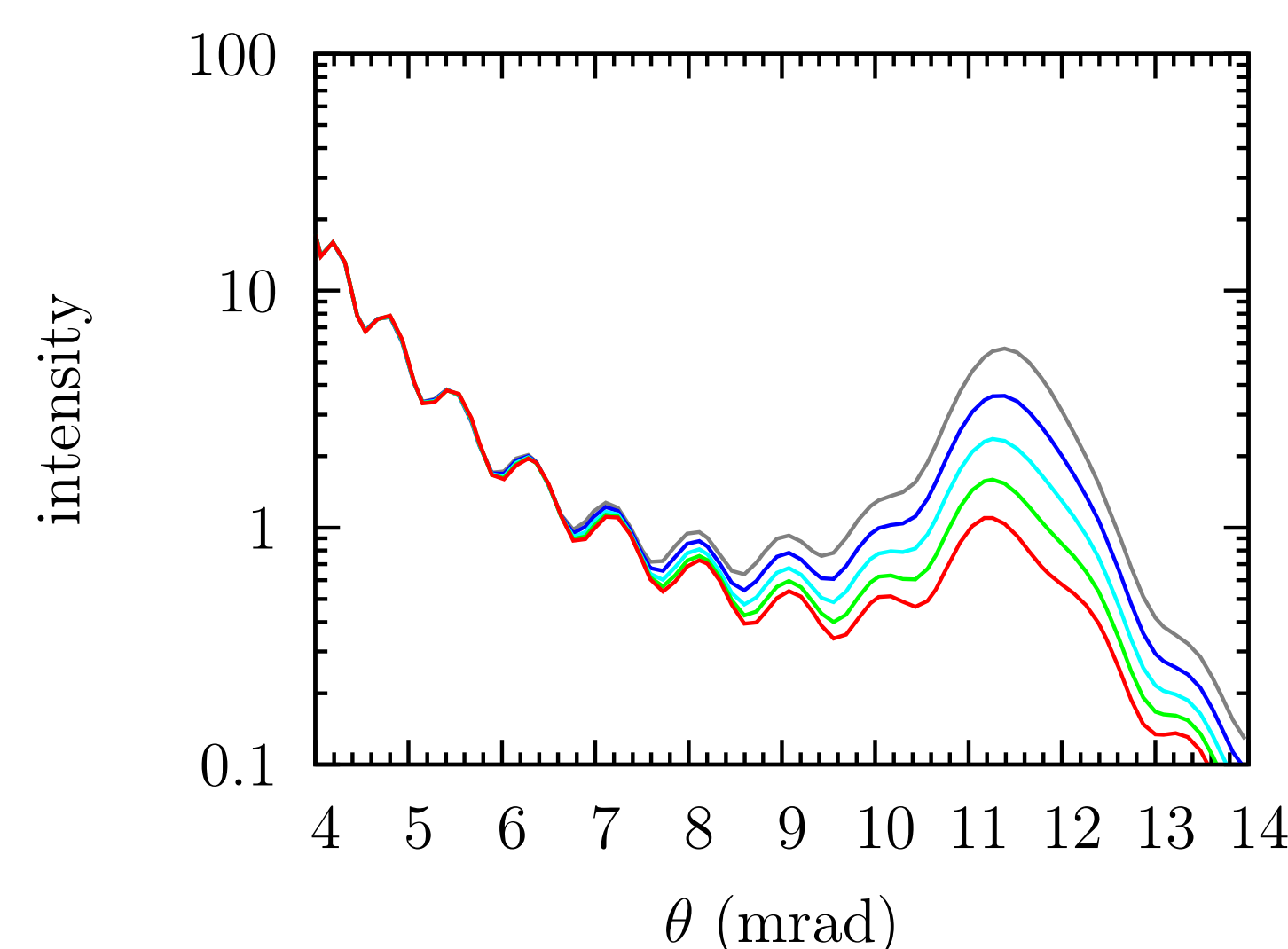
For the activation energies of the diffusion along the  $a$ -axis we found  $E_A = (2.0 \pm 0.3) \text{ eV}$ . The pre-exponential factor of diffusion gives  $D_0 = (1.43 \pm 0.4) \cdot 10^{10} \text{ nm}^2\text{s}^{-1}$ , which is rather low for diffusion in crystalline solids. In the figure below the open triangular/circular points are the results of the kinematical/dynamical theory for the  $(a+c)$ -axis and the filled points are the final results for the  $a$ - and  $c$ -axis.



## KINEMATICAL/DYNAMICAL THEORY

We concluded for our strongly absorbing samples (Pt), that the dynamical effects amount to a significant correction in the diffusion coefficient. In materials with a high density of resonant scattering centers and low absorption, therefore the application of the dynamical theory for the determination of the diffusion coefficients is inevitable.

In the case of an  $^{57}\text{Fe}/^{\text{nat}}\text{Fe}$  multilayer the difference between the kinematical/dynamical evaluation is of the order of 80%. This was concluded from the simulated intensities below.



## REFERENCES

- [1] M. Rennhofer et al., Phys. Rev. B **74** (10), 104301 (2006)
- [2] M.A. Andreeva, N.G. Monina, S. Stankov, Moscow Univ. Bull. **63** (2), 132–136 (2008)
- [3] W. Sturhahn, E. Gerdau, Phys. Rev. B **49**, 9285–9294