Streumethoden zur Untersuchung komplexer (biologischer) Materialien

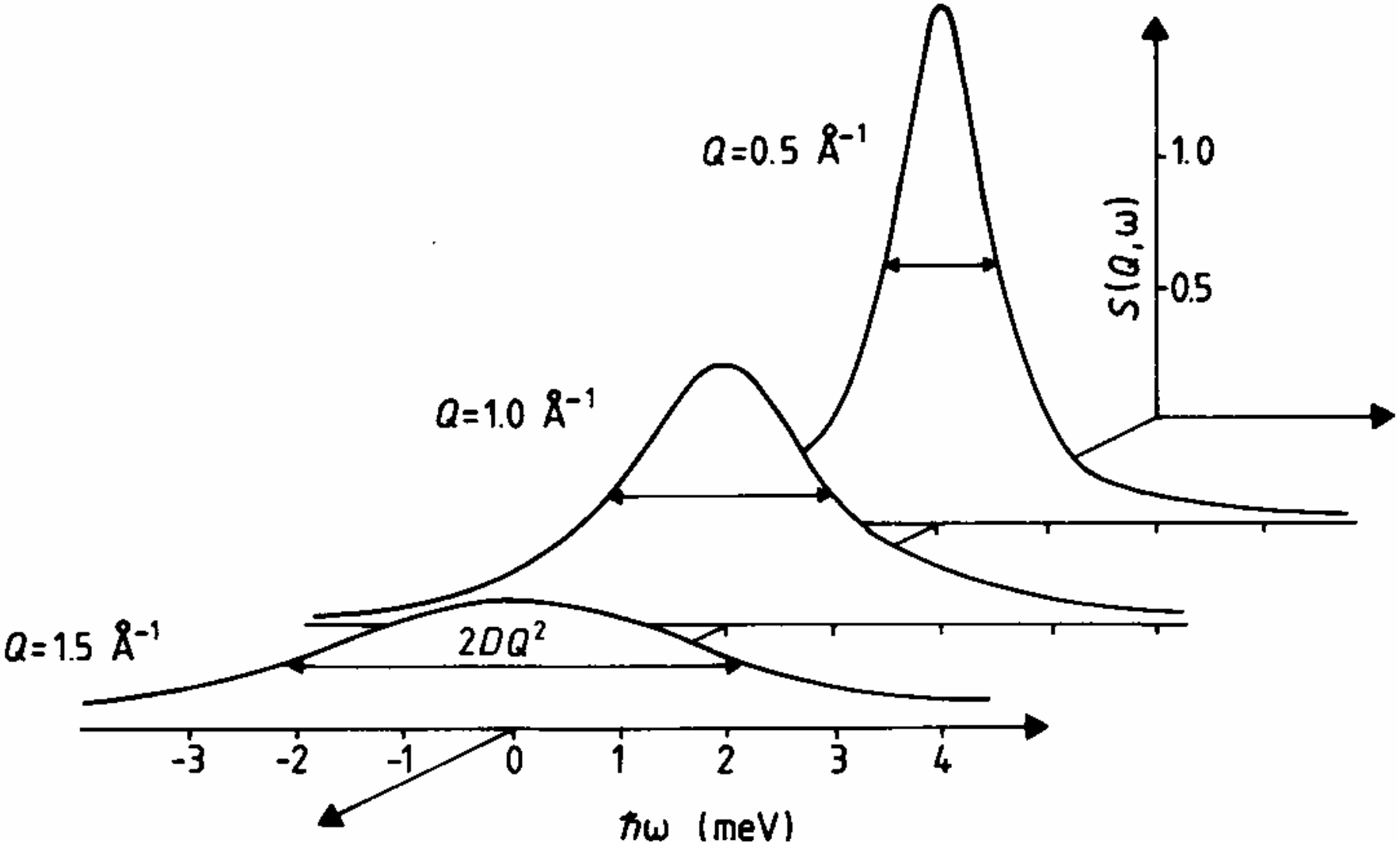
4. Erzeugung von Röntgenstrahlung

5. Neutronenquellen

6. Diffusion in kondensierter Materie: Quasielastische Neutronenstreuung
6.1 Allgemeines
6.2 QENS zur Untersuchung von Translations- und Rotationsdiffusion [Igor]
6.3 Instrumentierung: Neutronen-Spektrometer [heute: Rückstreuung]
6.4 Beispiele zur QENS an biologischen Materialien

7. Röntgen-Absorptions-Feinstruktur-Spektroskopie (XAFS)

Streufunktion bei Translationsdiffusion



Bée 1988, Fig. 5.2

QENS an flüssigem Argon

kohärente Effekte!

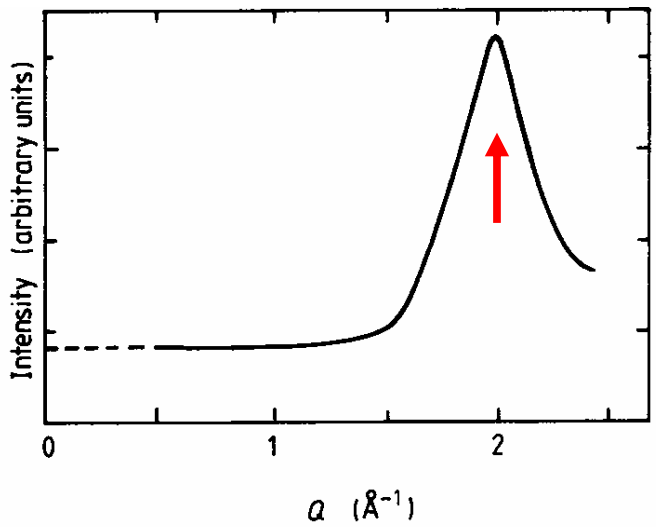


Figure 5.3 Diffraction pattern of liquid agron obtained with a wavelength of 4 Å (Dasannacharya and Rao 1965).

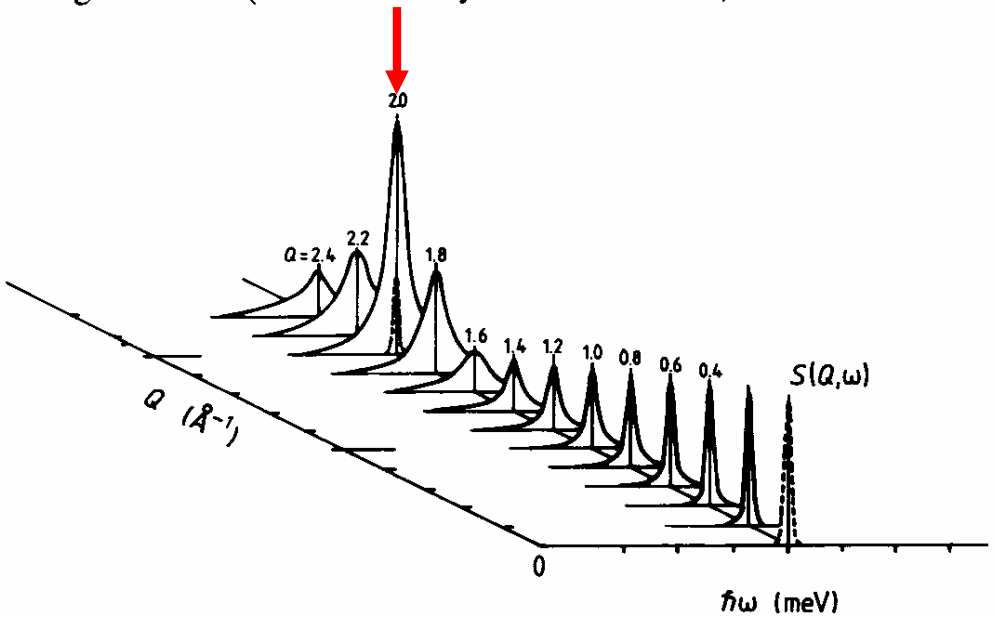
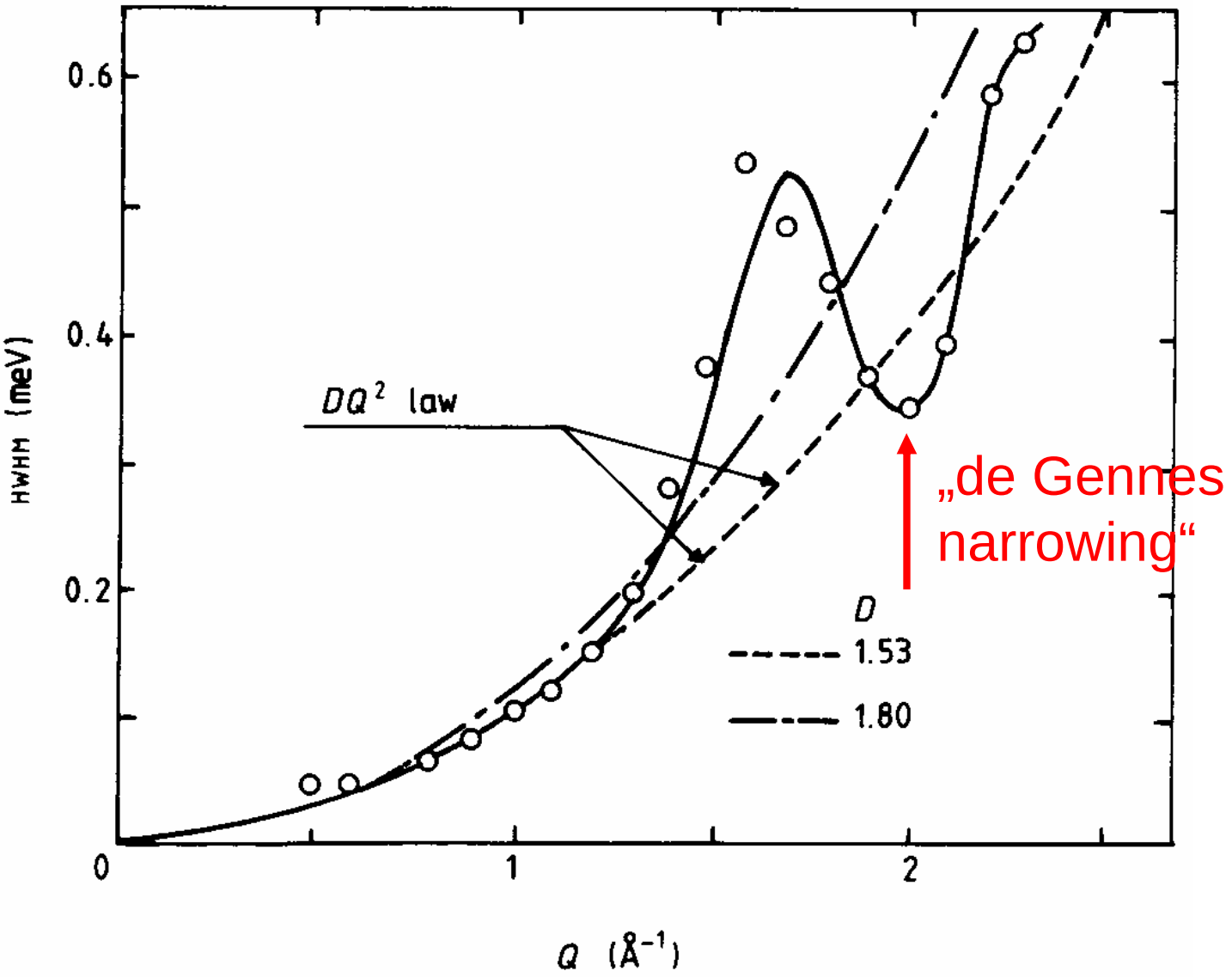


Figure 5.4 The scattered intensity for liquid argon plotted as a function of wavevector transfer Q and energy transfer $\hbar\omega$ (the dotted line represents the resolution function).

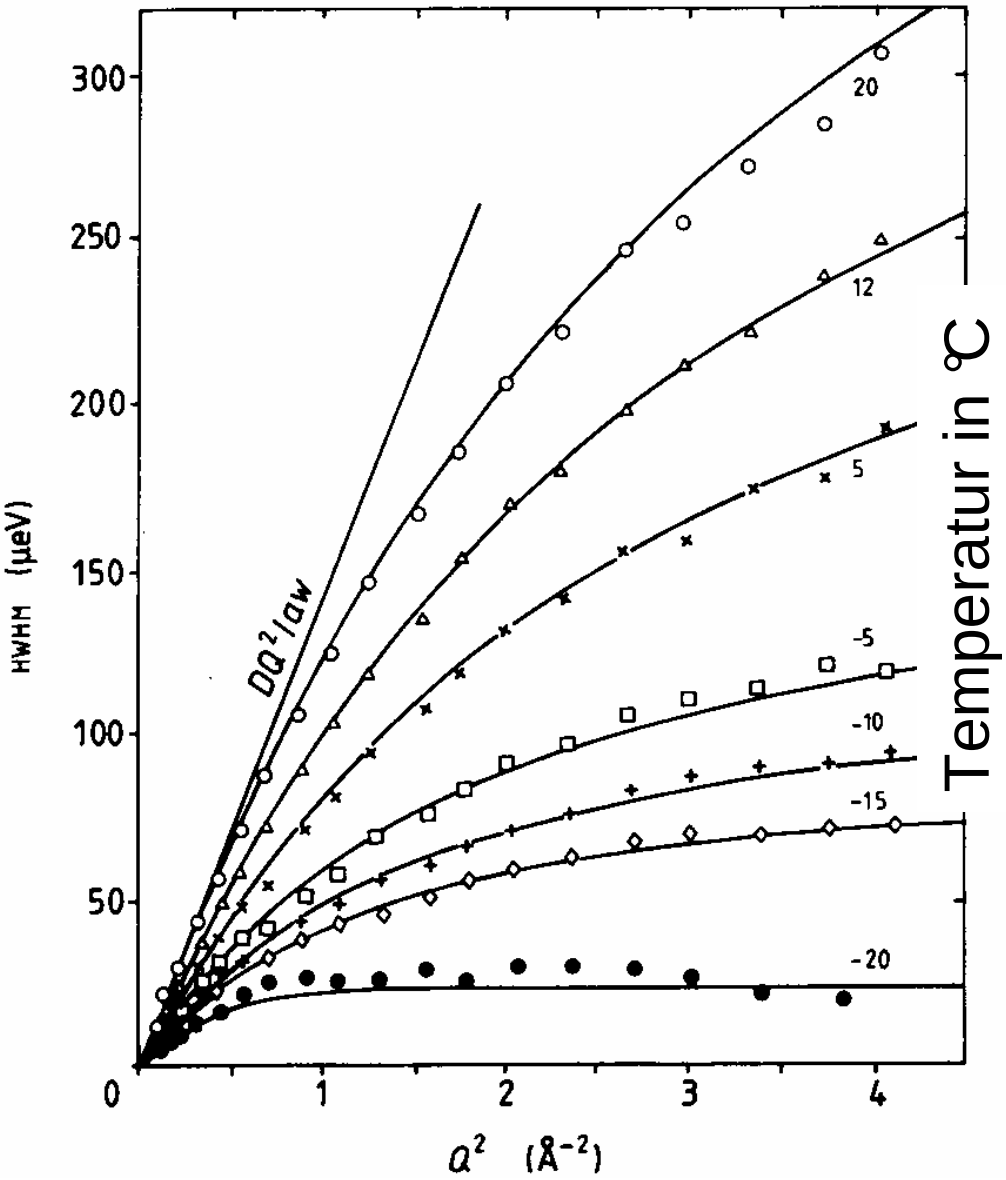
Bée 1988

QENS an flüssigem Argon



Bée 1988, Fig. 5.5

Translationsdiffusion von Wasser

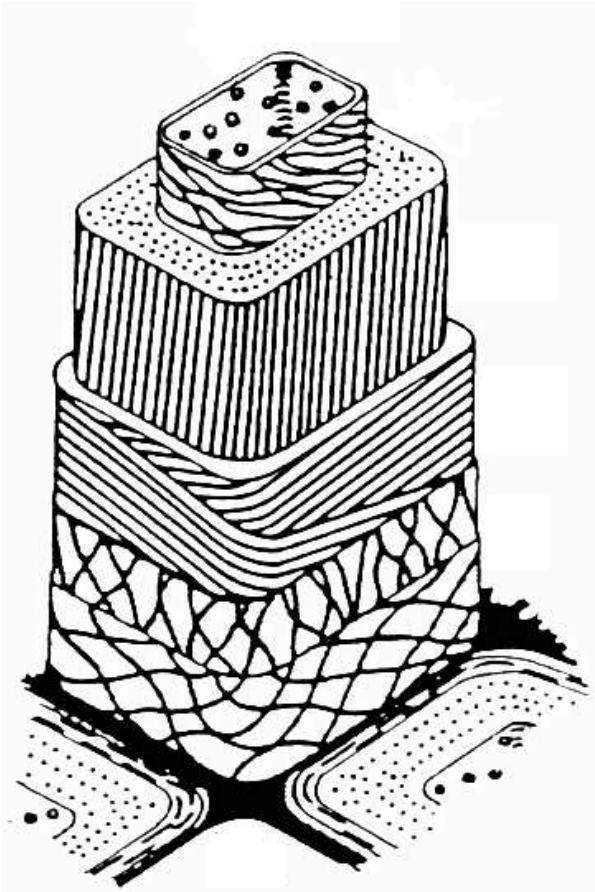


Wasser:

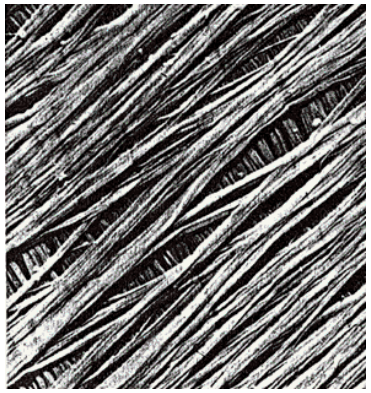
- auch Rotationsdynamik
- „Käfige“ durch H-Brücken

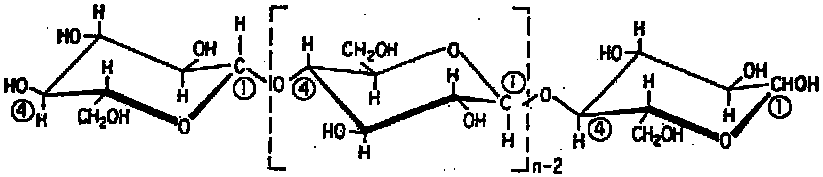
Bée 1988, Fig. 5.12

Cellulose in plant cell walls



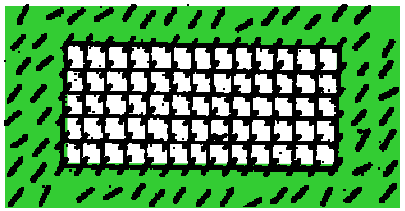
wood cell



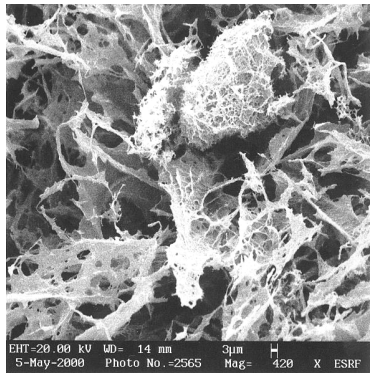


Cellulose *microfibrils*
= nanocrystals

Water adsorption to disordered regions
breaks up hydrogen bonds

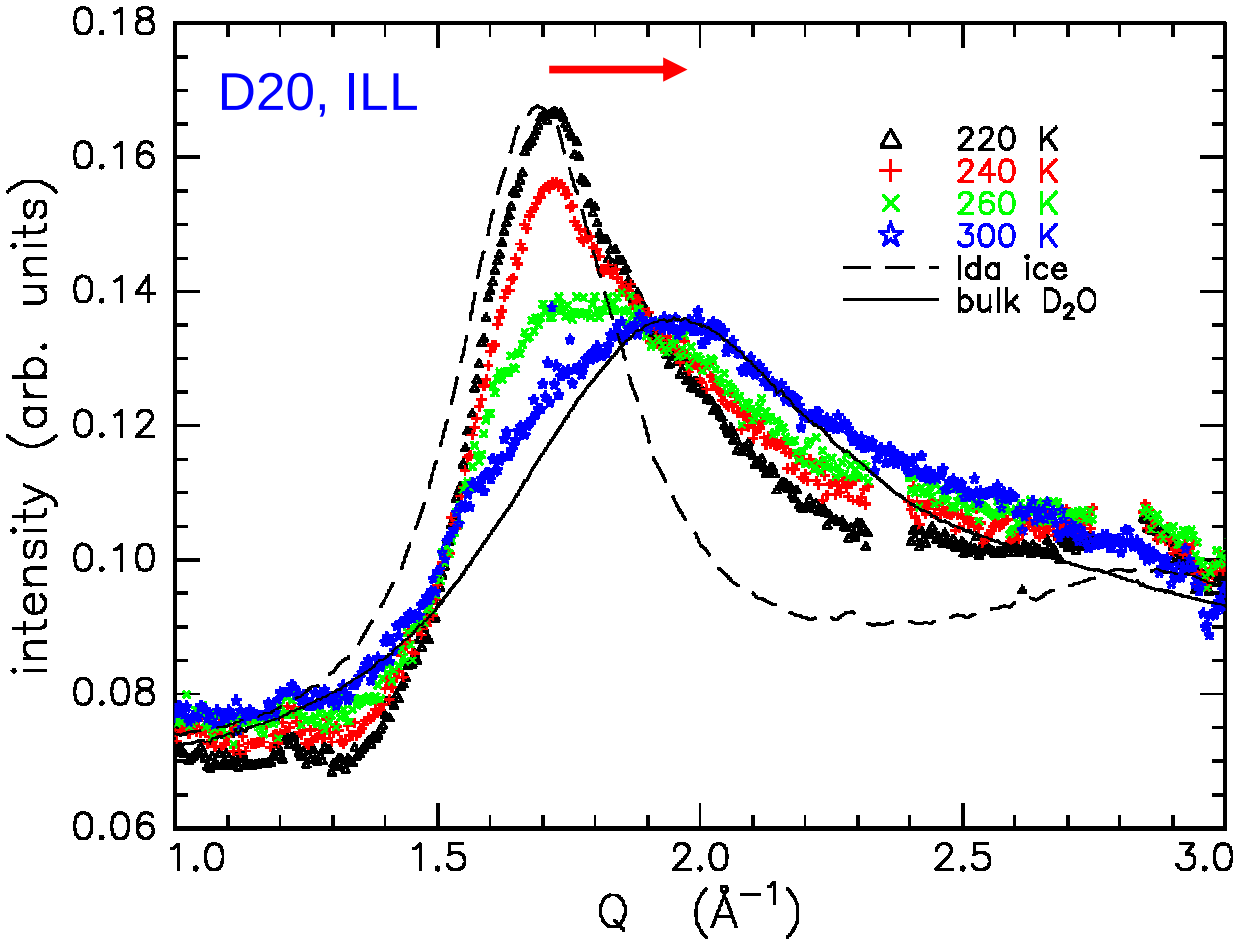


model system:
amorphous cellulose!



M. Müller, C. Czihak, H. Schober, Y. Nishiyama, G. Vogl
Macromolecules **33**, 1834-1840 (2000)

Structure of adsorbed water

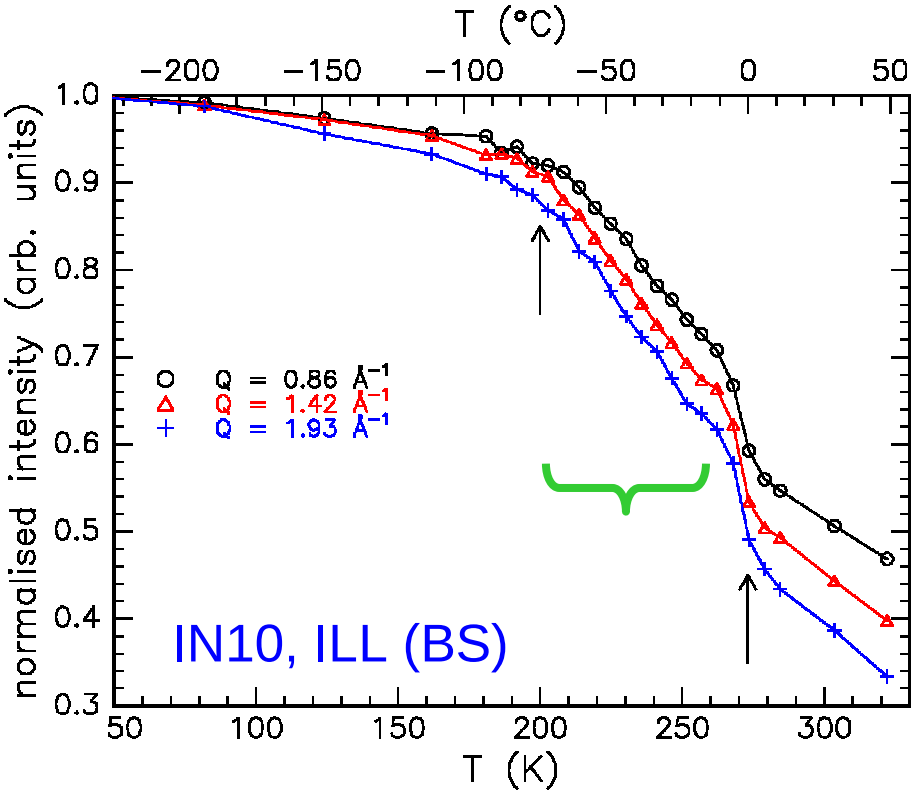


temperature-dependent change of *S(Q)*:

- glass transition?
- heterogeneous melting?

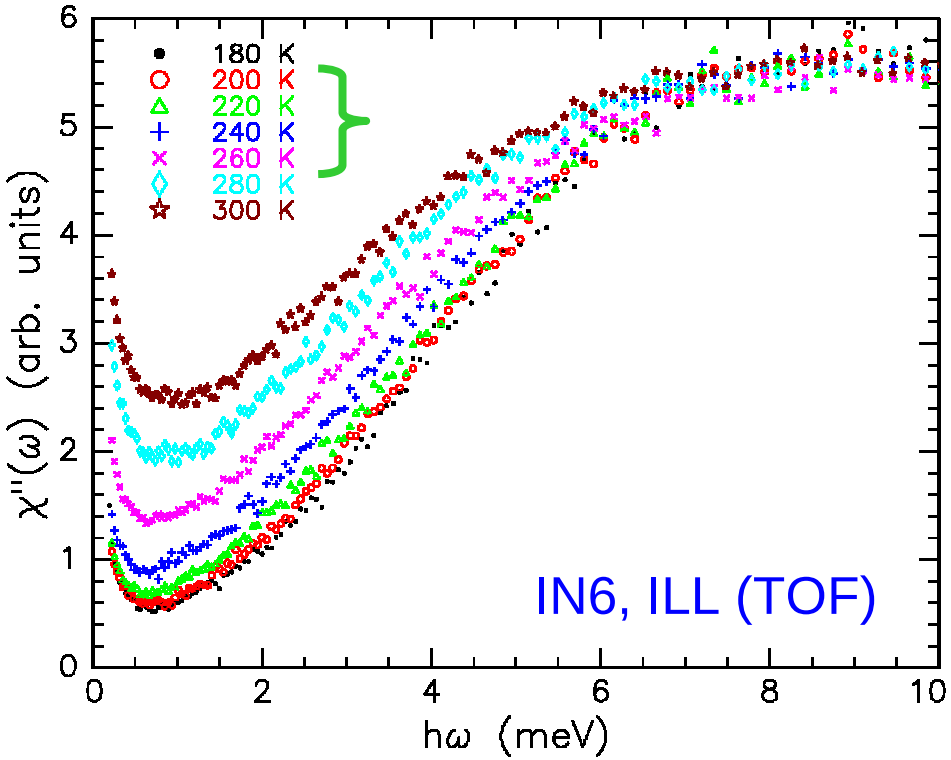
What about dynamics?

Dynamics of adsorbed water



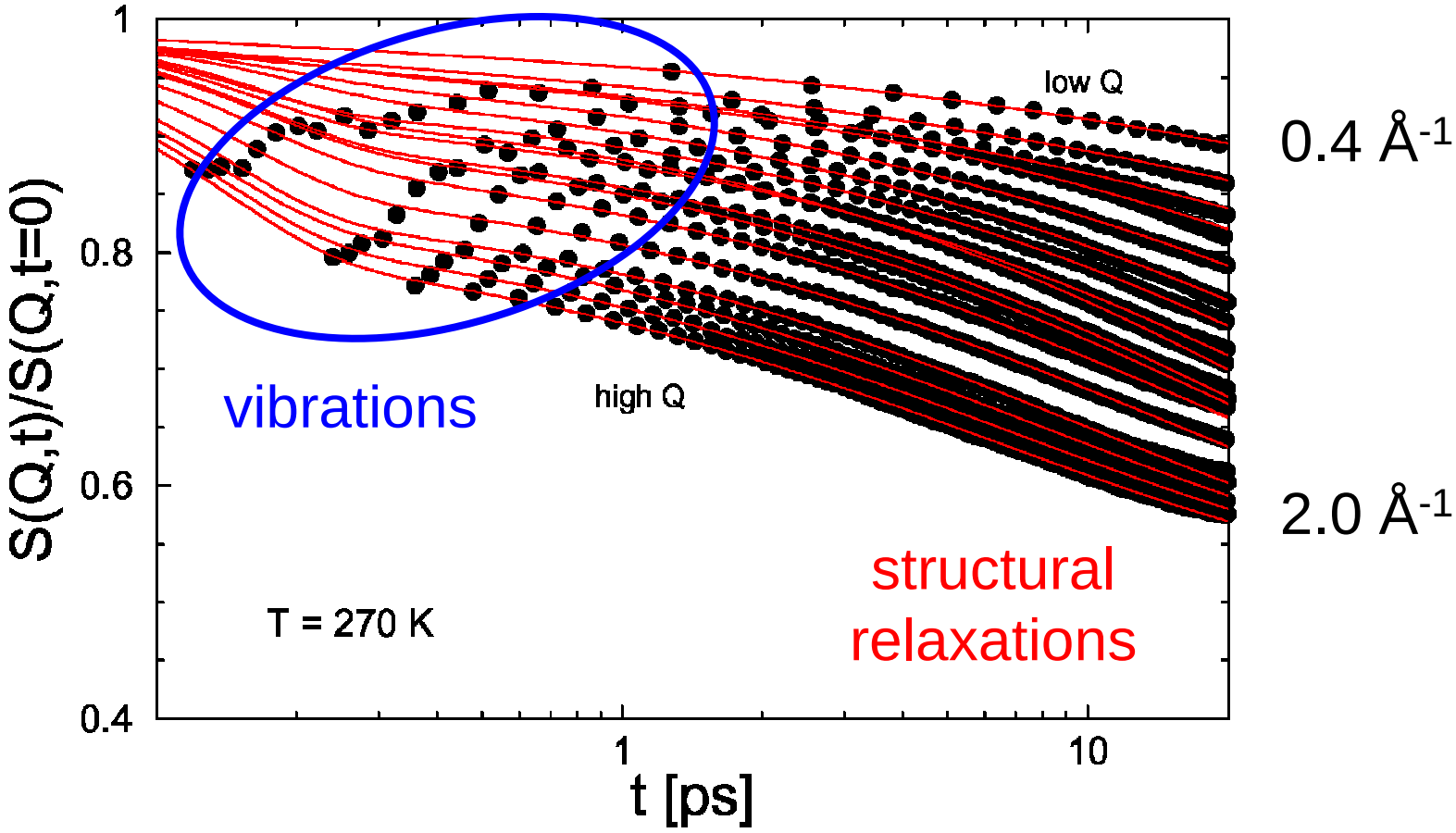
onset of dynamics at 200 K,

never in the ns time window



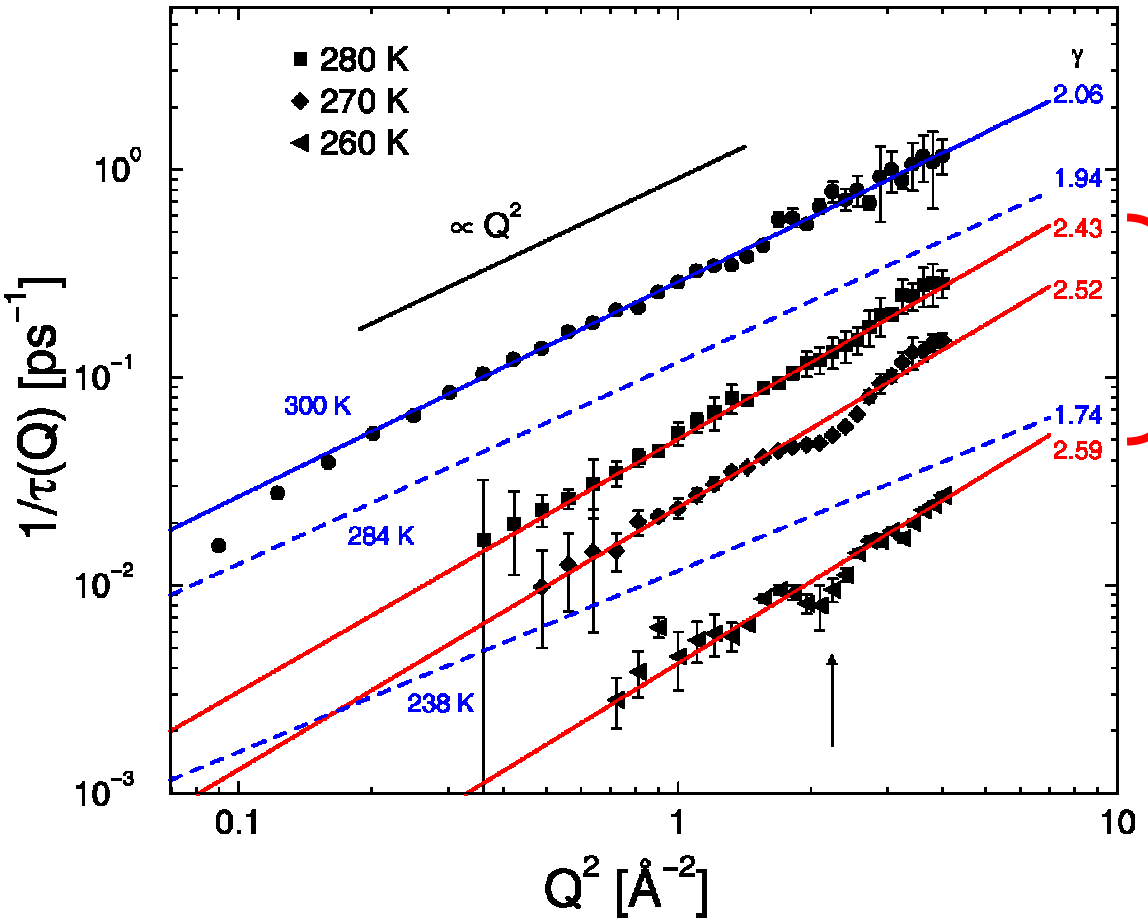
Model fitting

- 2 Lorentzians: no good fit ⇒ *coupled* rotation & translation
- model for supercooled water* applied to data



*S. H. Chen, C. Liao, F. Sciortino, P. Gallo, P. Tartaglia
Phys. Rev. E **59**, 6708-6714 (1999)

Structural relaxations of supercooled water in cellulose



bulk water

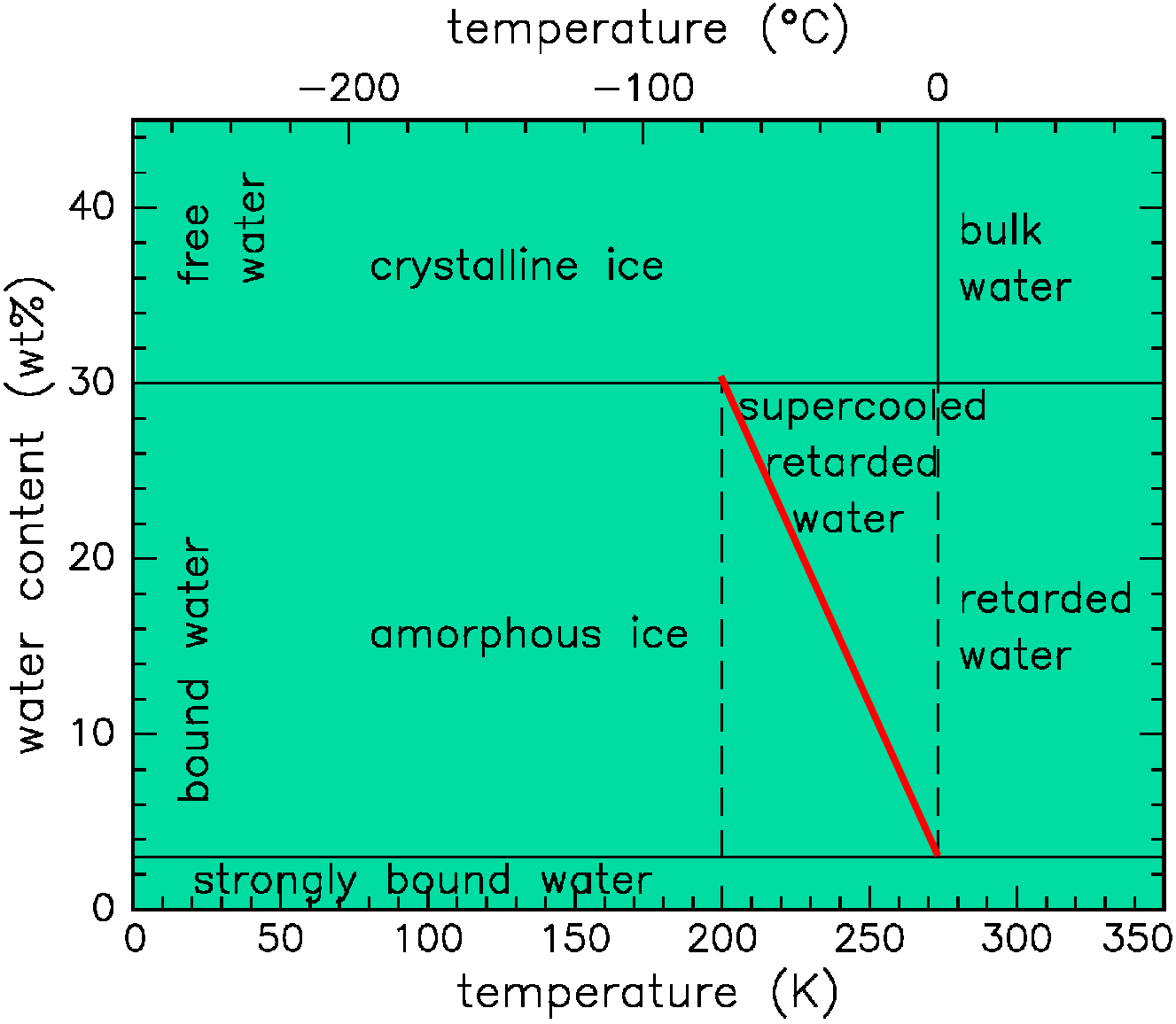
water adsorbed to cellulose

power law $\tau^{-1} \propto Q^{\gamma}$

diffusion at 270 K about *6 times slower* than in bulk water

C. Czihak, M. Müller, H. Schober, G. Vogl
Journal de Physique IV - Proceedings **10**, 199-202 (2000)

Phase diagram of adsorbed water

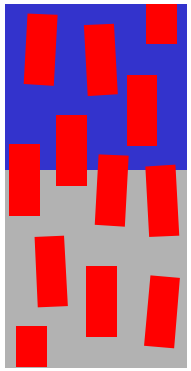


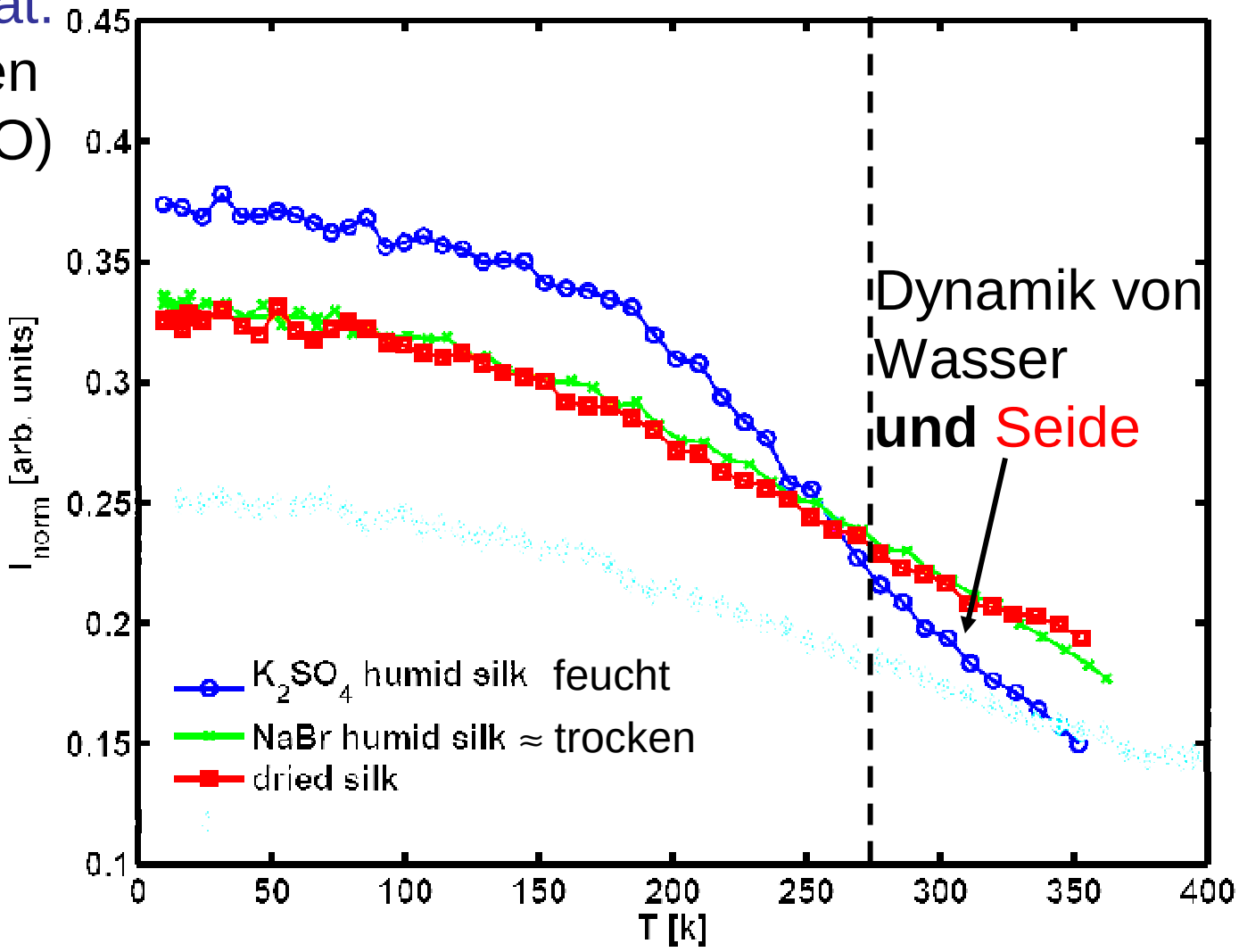
M. Müller, C.Czihak, H. Schober, G. Vogl
unpublished

Dynamik von Wasser und Seide

Seide: Proteinfaser (Fibroin); ebenfalls kristalline Anteile

höhere Intensität:
mehr Protonen
(H_2O)





T. Seydel, C. Dicko, M. Müller (2007)