ESRF	**Experiment title: High-frequency dynamics of oriented DNA studied by inelastic X-ray scattering**	**Experiment number**: SC-1236
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Report:

Films of oriented deoxyribonucleic acid (DNA), prepared by the wet spinning method, have been studied using inelastic x-ray scattering [1]. Spectra were recorded within the range of energy transfers $-30 < \hbar\omega < 30$meV at momentum transfers $\hbar\mathbf{Q}$ ranging from 2.5 to 30 nm^{-1} whereby the direction of **Q** essentially coincided with the helical axis. Measurements at ambient temperature cover samples in the A,B,C, and D conformations of DNA. Within the limits of the instrumental resolution of 1.8 meV, the spectra were analysed by the response of a damped harmonic oscillator delivering dispersion and damping of modes having displacements with nonzero projections onto **Q**, i.e. essentially the compression waves travelling along the helical axis. The longitudinal speed of sound resulting from the sinusoidal dispersion varies only weakly with conformation (see Table 1). The dispersion curves exhibit a minimum at about the inverse rise per residue, which – together with strong elastic scattering - reflect the large degree of disorder. Overdamping of the modes is observed for $Q > 5$ nm^{-1} (see Figure 1).

Conformation	sound velocity [m/s]	Sound damping [meV]
A	2880+/-100	$0.98 \times Q^{1.27}$
B	2830+/-50	$1.04 \times Q^{1.30}$
C	2925+/-100	$0.87 \times Q^{1.33}$
D	2985+/-50	$0.98 \times Q^{1.28}$

Table 1: Sound velocities and Q dependence of sound damping, G(Q), for the four DNA conformations at ambient temperature.

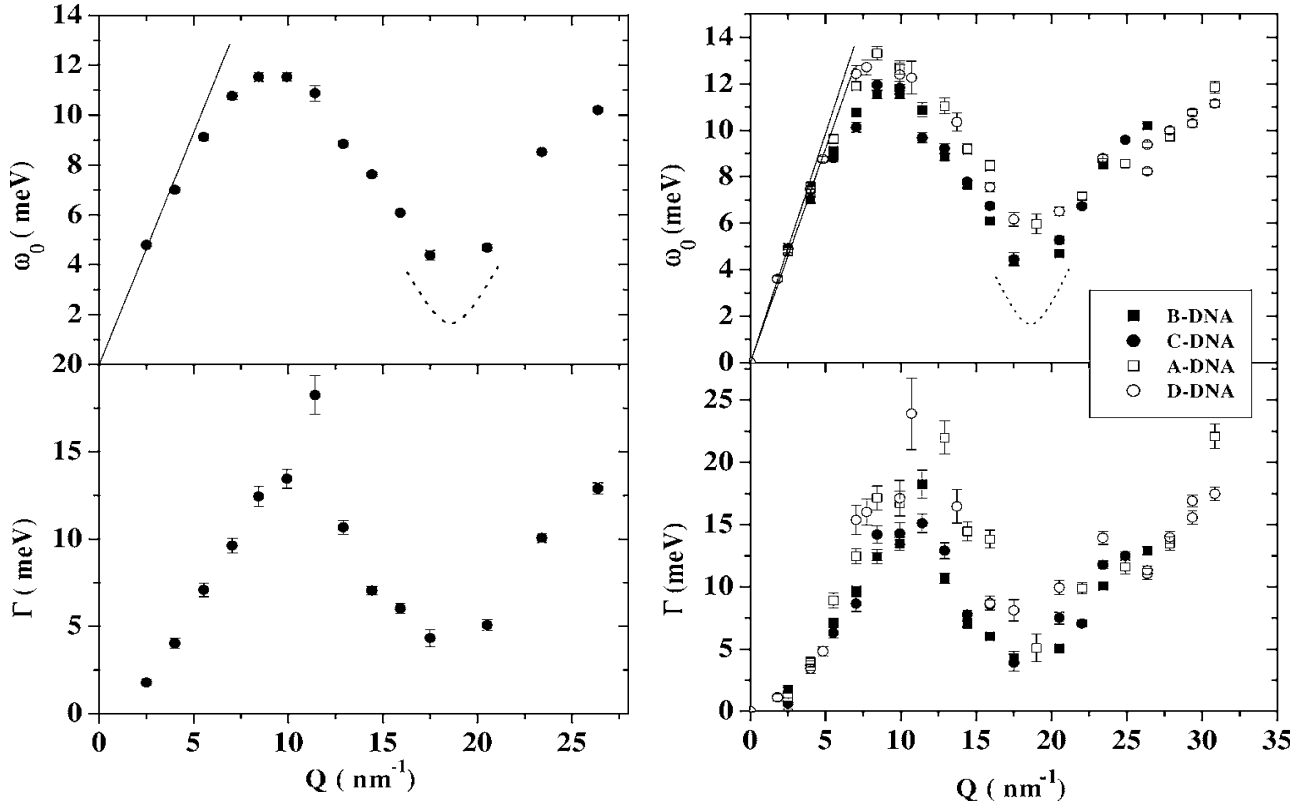

Figure 1: Dispersion and eigenfrequency ω_0 and damping Γ of the damped harmonic oscillator ansatz for B-DNA (left panel) and all four conformations (right panel) at ambient temperature. The initial slopes, corresponding to the respective sound velocities, are indicated by thin, straight lines. The dotted hyperbola represents results obtained by neutron scattering [2].

The dispersion and sound damping of B-DNA has been analysed using two simplified models, i.e., the modes of a simplified double helix [3] and the effect of disorder on the dispersion of a linear chain [4,5]. The first model suggests that the LA- and a breathing branch should be observed within the first Brillouin zone. Within the experimental resolution, however, we observe neither an indication of a bimodal spectral response nor a deviation from the effective sinusoidal dispersion. In the second Brillouin zone, however, one might conclude that the experimentally determined DHO-parameters represent an effective average over the response due to the LA- and breathing branch. The second model describes well the sinusoidal dispersion, but it fails to reproduce the observed damping by one order of magnitude.

The limits of interpreting the observed large damping parameters in terms of either unresolved dispersion branches or disorder within the quasi-crystalline approximation suggest the inclusion of both strong anharmonicity and finite coherence length of modes in modelling the low frequency excitations of DNA. It is tempting to associate the large damping with the strong anharmonicity of the effective Morse potential of the hydrogen bonds between nucleic acid pairs. An extension of the modelling approach of Cocco and Monasson [6] to all dominating external degrees of freedom seems highly desirable.

References

[1] M. Krisch, A. Mermet, H. Grimm, V.T. Forsyth, and A. Rupprecht; Phys. Rev. E 73, 061909 (2006).
[2] H. Grimm et al.; Phys. Rev. Lett. 59, 1780 (1987).
[3] H.Capellmann and W.Biem, Z.Physik 209, 276 (1968).
[4] I.Ishida and T.Matsubara, J.Phys.Soc.Japan 38, 534 (1975).
[5] P.Kleinert, and R.Leihkauf, phys.stat.sol.(b) 97, 491 (1980).
[6] S.Cocco, and R.Monasson, J.Chem.Phys. 112, 10017 (2000).