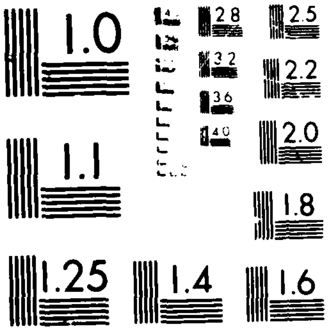
AD-A187 163   MICROWAVE INTERACTION WITH DNA IN SOLUTION(U) PURDUE   1/1
UNIV LAFAYETTE IND DEPT OF PHYSICS L L VAN ZANDT
10 OCT 87 N00014-85-K-0401

UNCLASSIFIED   F/G 6/1   NL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SECURITY CLASSIFICATION OF THIS PAGE

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REPORT DOCUMENTATION PAGE

AD-A187 163

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1b RESTRICTIVE MARKINGS
NA

3 DISTRIBUTION / AVAILABILITY OF REPORT
Distribution Unlimited

2b DECLASSIFICATION / DOWNGRADING SCHEDULE
NA

4 PERFORMING ORGANIZATION REPORT NUMBER(S)
NA

5 MONITORING ORGANIZATION REPORT NUMBER(S)
NA

6a NAME OF PERFORMING ORGANIZATION
Purdue University

6b OFFICE SYMBOL (If applicable)
NA

7a NAME OF MONITORING ORGANIZATION
Office of Naval Research

6c ADDRESS (City, State, and ZIP Code)
Department of Physics
W. Lafayette, Ind 47906

7b ADDRESS (City, State, and ZIP Code)
800 N. Quincy St.
Arlington, Va 22217

8a NAME OF FUNDING / SPONSORING ORGANIZATION
Office of Naval Research

8b OFFICE SYMBOL (If applicable)
ONR

9 PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER
N00014-84-K-0401

8c ADDRESS (City, State, and ZIP Code)
800 N.Quincy St.
Arlington, Va 22217

10 SOURCE OF FUNDING NUMBERS

PROGRAM ELEMENT NO	PROJECT NO	TASK NO	WORK UNIT ACCESSION NO
61153N	RR04108		

11 TITLE (Include Security Classification)
(U) Microwave Interaction with DNA in Solution

12 PERSONAL AUTHOR(S)
Van Zandt, Lonnie L.

13a TYPE OF REPORT
Final

13b TIME COVERED
FROM 5/85 TO 9/87

14 DATE OF REPORT (Year, Month, Day)
87/Oct/30

15 PAGE COUNT
4

16 SUPPLEMENTARY NOTATION

17 COSATI CODES

FIELD	GROUP	SUB-GROUP
08		

18 SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
DNA;counterions,resonance,microwaves

19 ABSTRACT (Continue on reverse if necessary and identify by block number)

DNA polymer in aqueous solution responds to microwave illumination. Depending on the nature of the solvent in the immediate vicinity of the molecule, long lived resonances may be excited. These resonances correspond to standing compressional waves of varying frequencies on the polymer chain. Account is taken of the dielectric properties of the aqueous medium, ionic conductivity arising from dissolved salt, condensation of the salt ions near the polymer, and the variation of all the parameters with temperature and ion concentration.

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20 DISTRIBUTION / AVAILABILITY OF ABSTRACT
☒ UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT ☐ DTIC USERS

21 ABSTRACT SECURITY CLASSIFICATION
(U)

22a NAME OF RESPONSIBLE INDIVIDUAL
Dr. M. J. Marron

22b TELEPHONE (Include Area Code)
202/696-4055

22c OFFICE SYMBOL
ONR

DD FORM 1473, 84 MAR

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SECURITY CLASSIFICATION OF THIS PAGE

FINAL REPORT ON CONTRACT N00014-84-K-0401

Principal Investigator: L. L. Van Zandt

Contractor: Purdue University

Contract Title: Microwave interaction with DNA in Solution

Start Date: May 15, 1985

Research Objective: To ascertain the physical parameters of DNA in saline solution for which resonant absorption of microwave illumination could be expected; to extend the parameter evaluation so that microwave absorption studies can become a tool for examining the interaction between DNA polymer and its solvent.

Progress: A detailed theory of the interaction of DNA polymer, aqueous solvent, and microwave illumination has been developed. This theory includes the effect of the redistribution of dissolved salt ions around the immediate neighborhood of the charged polymer molecule as well as their motion in response to the microwave field. The effects of varying temperature and varying salt concentration were studied.

The motion of DNA in response to an outside driving field depends upon the charged nature of the polymer molecule, the elasticity of the molecule, the distribution and mobility of surrounding charges - counterions - the elastic and viscous properties of the surrounding solvent bath, and the detailed configurations of the electric and magnetic fields acting on the molecule. This last dependence also introduces the dielectric properties of the water into the combined interaction. Altogether, nine coupled second order differential equations had to be solved to obtain a convincing solution to this entangled system. In these equations, the solution of each equation provided a field that served as the inhomogeneous term for succeeding differential equations. The full details of this calculation are inappropriate for a report of this nature; they are being reported elsewhere and will not be elaborated here.

Of particular interest for the performance of this calculation is the nature of the mechanical structure of the water in the immediate neighborhood of the polymer. Because of the strongly charged nature of DNA and the polar nature of the water molecule, it is to be expected that a substantial modification of the mechanical behavior of the near water would occur. This modification or "structuring" is a feature of the first few molecular monolayers of water surrounding the polymer. In effect, the DNA is surrounded by a sheath of a third type of material.

We found that the resonance behavior of DNA, or the lack of it, is strongly influenced by the properties of this sheath, and also by the nature of the coupling between the inner surface of the sheath and the enclosed, "dry" polymer. We calculated absorption spectra for a wide range of properties of this sheath and its interaction with the DNA. Of special interest in this regard were the experiments of Edwards, Davis, Saffer & Swicord in which a series of well defined resonances were found. The resonances of this experiment corresponded well with those to be expected on the grounds of earlier theoretical investigations of the normal modes of vibration of DNA chains and also wi Brillouin scattering experiments on dry DNA fibers.

In this contract, we found that the interpretation of the EDSS experimental resonances required a rather small but not unimaginably small coupling of the polymer to the structured water sheath. In the exposition of this calculation referred to above, we give reasons why the coupling might have so small values as the experiments seemed to require. It should be noted, however, that the experiments have recently been seriously challanged by others who have been unable to reproduce the EDSS results. The resonances may not ultimately stand the test of history.

Our analysis shows, however, that as one proceeds to the higher range of microwave frequencies, eventually sharp resonances must become visible. This is a consequence of the concordance of two time scales; the finite lifetime of weak binding interactions between pairs of water molecules, substantially shorter than typical microwave periods, eventually becomes comparable to or longer than the oscillation period as the frequency rises. As one exceeds this characteristic frequency, the mechanical properties of water must change. This is the well known "liquid-glass transition".

A corresponding transition in the interaction properties of the polymer molecule and its surrounding sheath of structures water must also occur. The principal achievement of this work is the demonstration that the microwave DNA interaction features must be dominated and determined by the nature of this polymer-sheath interaction. In this regard, the recent measurements of Lindsay on moderately wet DNA fibers are of crucial interest because they seem to show a much longer characteristic lifetime of polymer-sheath interactions leading to a transition in the system properties analogous to the liquid-glass transition at at least an order of magnitude lower frequency than for the pure water case. The structural features in our results are a consequence of this lowering of the transition frequency.

We also applied the formalism and the corresponding computer code to the case of various temperatures and various concentrations of salt in the solvent medium. Some dependence in the frequency locations of the structural features and their amplitudes was noted in each case. A very curious accidental cancellation of effects occurs in the case of the temperature dependence of the absorption. When account is taken of the temperature dependence of the bulk water viscosity and dielectric constant, the spectral features we calculate become almost completely temperature independent. We verified that this temperature "non-dependence" is in fact the result of competing effects, each of which by itself results in substantial variation of properties.

Publications:

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[4] Resonant Microwave Absorption by Dissolved DNA, L.L. Van Zandt, Phys Rev Lett. 57, 2085 (1986).

[5] Why Structured Water Causes Sharp Absorption by DNA at Microwave Frequencies, Jour. Biomol. Struc. & Dyn. 4, 569 (1987).

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[7] Response of DNA in Aqueous Solution to Microwave Irradiation, M.E. Davis & L.L. Van Zandt, Jour. Biomol. Struc. & Dyn., submitted, (1988).

[8] Theory of the Response by DNA in Solution to Microwave Illumination, M.E. Davis, theses, Purdue University (1987).

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