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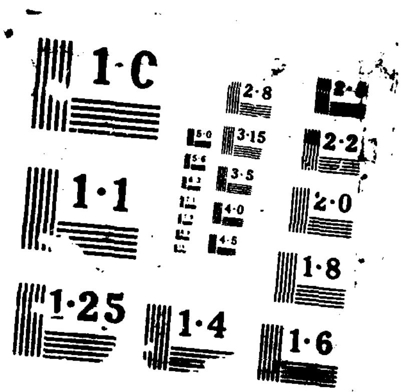
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18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number): DNA HELIX MELTING, Deoxyribonucleic Acid, FREE ELECTRON LASER IRRADIATION

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

We have calculated the far infrared absorption for several models of double helical DNA. These results are in good agreement with experimental observations. We have also fitted our results to observed inelastic neutron scattering data. Again the results are in excellent agreement with observation. We have extended our calculations on helix strand melting to include methylated DNA and many other DNA's of varying base pair sequence. All of the results are useful in leading to more precise predictions of the dynamics of DNA strand separation in a far infrared radiation field. We have also extended our model so as to predict energy flow in the natural process of DNA transcription.

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22a. NAME OF RESPONSIBLE INDIVIDUAL: Charles L. Houston, III, Captain USAF

22b. TELEPHONE (Include Area Code): (202)-693-1556

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PROGRESS AND ANNUAL REPORT ON CONTRACT N00014-86-K-0252

PRINCIPAL INVESTIGATOR: E. W. Prohofsky

CONTRACTOR: Purdue Research Foundation

CONTRACT TITLE: A Spectroscopy of Helix Melting

START DATE: 1 April 1986

RESEARCH OBJECTIVE: To investigate the role of far infrared excitations that can be excited by FEL radiation, in the melting of DNA: to develop an understanding of the role of such excitations in transcription and replication.

PROGRESS (Year 2): We have made considerable progress toward a calculation of the amount of energy in a free electron laser beam that would actually be absorbed by DNA. The first step required a careful fit of our calculated spectrum to infrared absorption observations. This has been completed and the fit is detailed in the manuscript "Calculation of Far Infrared Absorption in B poly(dA)•poly(dT) which is enclosed as a technical report. We find that the actual absorption strength does depend on the state of aggregation of the DNA i.e., there are strong interhelical effects. More sophisticated calculations are needed to accurately model the true absorption and we are proceeding with such calculations.

We have been able to fit our basic vibrational mode model to newly published inelastic neutron scattering observations. We find that our model fits the observations very well. We have used the information obtained to improve our model by allowing us to separate charge effects from dielectric constant effects in a more complete manner. The reason for this is the inelastic neutron data is at high enough frequencies to be above the large rapidly changing dielectric response of water. I enclose two manuscripts on this subject as technical reports.

We have made progress on investigating the role of base pair sequence in DNA melting. We have also studied sequence dependent response to far infrared absorption. We have calculated the melting behavior differences for methylated vs. unmethylated DNA and we have calculated the melting behavior for Z conformation DNA. For the methylation case we predict a 7K increase in melting temperature for methylated Z-poly(dGC)•poly(dGC) compared to unmethylated B poly(dGC)•poly (dGC). The experimentally observed increase is 6K. The work on this melting variation is contained in three manuscripts which are enclosed as technical reports.

We have also explored the nonlinearity of the far infrared modes involved in melting and FEL absorption. We found that these modes are likely to display solitary wave narrowing which will be important in more detailed analysis of the effects of FEL irradiation. This work is detailed in a manuscript enclosed as a technical report.

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WORK PLAN (Year 3): We plan to continue along the lines of progress for the first two years. We will explore further the effect of state of aggregation on the actual far infrared absorption. When this is understood we can predict quantitatively the results of FEL irradiation on DNA. We plan to study absorption for helices in a crystal interacting with other helices. We plan to complete our study of base pair sequence effects on melting and far infrared absorption. Much of this effort has been completed but a manuscript of the comparison across the board will have to wait until we have a better handle on the melting of A-T base pair systems. We have also begun calculations on the transition from small amplitude normal mode behavior to large amplitude solitary wave behavior for these far infrared modes. We will continue such calculations in year three.

All of the efforts listed are key elements in the overall plan to study the absorption of FEL radiation and to predict the dynamic effects of that absorbed radiation. All of the individual elements in that program are progressing as outlined above. The task remaining is to complete the individual calculations and integrate the pieces to the analysis and prediction of the dynamical consequences of FEL radiation.

PUBLICATIONS AND REPORTS (Year 2):

1. L. Young and E. W. Prohofsky, "Calculation of Far Infrared Absorption in B poly(dA)·poly(dT) submitted for publication.

2. V. V. Prabhu, W. K. Schroll, L. L. Van Zandt, and E. W. Prohofsky. "Helical Lattice Vibrational Modes in DNA", to be published in Physical Review Letters.

3. W. K. Schroll, V. V. Prabhu, E. W. Prohofsky and L. L. Van Zandt, "Phonon Interpretation of Inelastic Neutron Scattering in DNA Crystals", submitted for publication.

4. X. M. Hua and E. W. Prohofsky "Vibrational Spectra of Double Helical Molecules with C_2 Symmetry," submitted for publication.

5. X. M. Hua and E. W. Prohofsky, "Normal Mode Calculation for Methylated Z-DNA poly(dG - m^5dC). (dG - m^5dC)", submitted for publication.

6. X. M. Hua, Y. Feng and E. W. Prohofsky, "Calculated Melting Temperature of Methylated Z-DNA", submitted for publication.

7. E. W. Prohofsky "Where Solitons May be Hiding in DNA and Their Possible Significance in RNA Transcription", submitted for publication

TRAINING ACTIVITIES: Two postdoctoral persons and five graduate students have had some level of support from this contract.

Women or minorities - 2

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