DOE-NSF-NIH Workshop on Opportunities in THz Science

February 12-14, 2004

Scope: Frequencies from 300 GHz to 20 THz

Science: Not engineering, not defense (can this be?)

Electrons, Diamonds, Nanomachines and Quantum Mechanics

Professor Bob Austin
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Dear Professor Austin:

You are invited to participate in the DOE–NSF–NIH Workshop on Opportunities in THz Science to be held February 12–14, 2004 at the Sheraton National Hotel in Arlington, VA. This workshop will explore opportunities in THz science broadly defined. One of the most important outputs of the workshop will be a report on scientific opportunities that are enabled by THz radiation .

There will be roughly 60 participants from the scientific community, along with about 20 representatives from government funding agencies. The questions that the co-organizers have been charged with are attached, as is the schedule of activities. Please note that this is a workshop, not a conference or symposium, and we are therefore asking for your active participation.

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Eric A. Rohlfing (DOE)

Janice Hicks (NSF, Chemistry)

Brenda Korte (NIH, Bioimagining)

.....and Gwyn Williams

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Charge questions:

- **What is the current status of THz applications in science?**

- **What is the current status of THz radiation sources, detectors and instrumentation?**
  Are scientific applications now limited by current source or instrumentation capabilities and, if so, how?
- **What new scientific opportunities are enabled by proposed new developments in THz sources and instrumentation?**
- **What are the characteristics of the source and instrumentation that are most important and relevant to the exciting new science?**
- **What is the size of the current user community for THz radiation?**
- What is the potential size of the community in the future, if new sources and instrumentation become available?
- What distribution of accelerator-based and table-top sources best meets the need of the current and potential user communities?
- What are the needs in THz detectors and instrumentation that will allow effective utilization of the new sources?

Are large-scale facilities or distributed centers of excellence most appropriate to serve the potential user community?

Materials I – semiconductor and insulators – Karl Unterrainer

Materials II – correlated-electron systems – Joe Orenstein

Physics – Bob Jones

Chemistry and Biology – Charles Schmuttenmaer

Medicine – Martyn Chamberlain

Breakout Session #1

Materials I – David Citrin
Materials II – Dimitri Basov
Physics – Tony Heinz
Chemistry and Biology – Bob Austin
Medicine – Warren Grundfest

2.1: Incoherent Synchrotron Radiation –Larry Carr

2.2: Coherent Synchrotron – Gwyn Williams (JLAB)

2.3: FELs (short pulse) – Lex Van der Meer (FELIX)

2.4: FELs (quasi-cw) – Jim Allen (UCSB)

Accelerator-based, Table-Top Sources – Sandra Biedron

2.5: Time-domain THz Spectroscopy – Ingrid Wilke

2.6: Time-resolved and High-Field THz Spectroscopy: Table-top Sources of HCP and Few-Cycle Pulses, also, Optical Pump/THz Probe Studies – Bart Noordham

2.7: Microwave Oscillators and Multplier Chains – Tom Crowe

2.8: THz QCLs – Qing Hu

2.9: Photomixers and PPLN (tunable narrowband) – Ted Norris

2.10: High Resolution Applications – Frank DeLucia

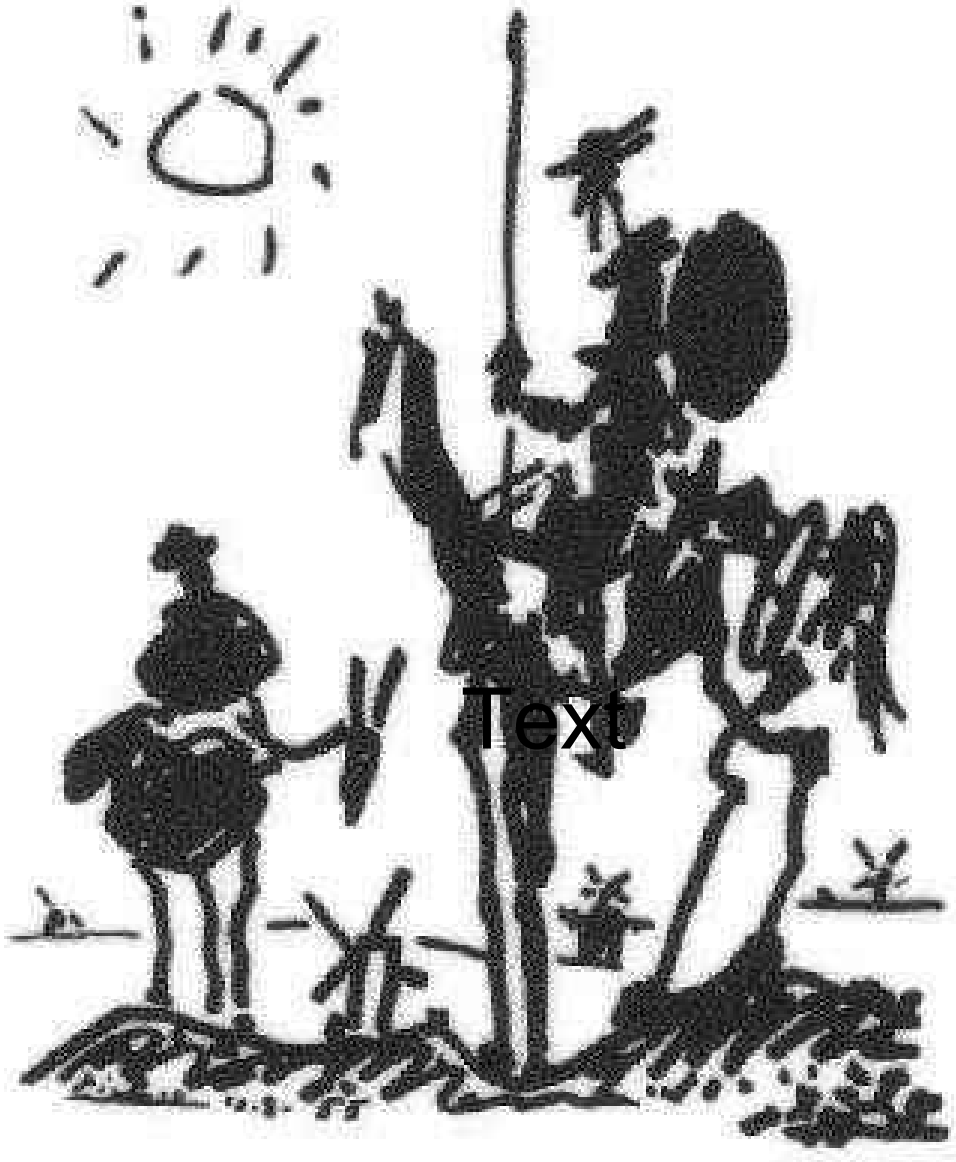
2.11: THz Imaging – X.-C. Zhang

Panel discussion to address:

1. Size of community, broken down by scientific field and by technique of choice;

2. Need for and advantages/disadvantages of: user-based facilities, centers of excellence (real or virtual), and single investigators and

3. Need for and useful form of a THz User's Network



Is it time for THz to Come Home?

"If we can speak of a "Holy Grail'' in biology and chemistry that represents a fundamental problem we would like to solve, it is the control of chemical reactions to do highly specific reactions. The control of specificity is of course something that biology does exceedingly well, and at present far exceeds the ability of chemists to accomplish. In order to do highly specific chemistry, it necessary for the energy put into a molecular system to not move into all degrees of freedom ergodically but instead to be channeled into a specific mode or small subset of modes. A related aspect to this question of mode control is the issue of how the solvent interacts with molecules at the ps time scale, in particular the role of water. We have only begun to explore this exciting area of basic science."

‘At the largest amplitudes, it may be possible to drive collective rearrangements of the lattice structure. Ions may be moved from their initial positions in the lattice, along selected lattice vibrational coordinates, into the positions they occupy in a different phase or domain orientation. In this limit a perturbative description of the spectroscopy will break down, and it will be more useful to think of the process in terms of THz coherent control over material structure. It should be within the realm of possibility to directly drive and control collective crystalline structure, and to monitor directly the collective transition from one structure to another. Careful control over the excitation conditions promises to reveal the dynamics of collective structural change.”

"We come to the issue of contrast imaging in cells. Although this properly belongs in the medicine section, we do need to stress that without an understanding of the basic mechanism of THz contrast mechanisms development of this this important technology will be hampered. Also, it may well turn out that THz spectroscopy of molecular complexes in the cell may provide an important window into ``label-free'' measurements of protein-protein interactions, of vital importance to the exponentially growing field of proteomics, the study of the expressed proteins in a cell and their interactions. The logic is, if in fact protein-protein interactions involved changes in the collective modes of the proteins, as one might expect since the proteins must change their conformations to bind in a specific manner, then differential THz spectroscopy of protein complexes may well turn out to be sensitive to the binding of proteins to each other. We know very little about this at present."

"A final comment: without the encouragement of advances in the theoretical community to calculate the response of molecules and materials to THz radiation, much of the experimental results that flow out of this work will lack a firm underpinning of understanding. This is a difficult area for theory: THz modes are collective in nature and involved the cooperative motions of many hundreds of atoms over time scales that begin in the ps domain and go out to the nanosecond domain. Conventional molecular dynamics treating a molecule as a set of classical balls a springs will not do for understanding these kinds of dynamics and the tools and computing power necessary for such studies should b developed."

"As we mentioned, a recent development has been Coherent Synchrotron Radiation. CSR is emitted from accelerated electrons when the electron bunch length is shorter than the wavelengths being emitted. Developments in a variety of accelerators have recently demonstrated sub-ps electron bunches which therefore emit CSR in the THz regime. This CSR emission is half cycle, high-power (uJ per pulse have been demonstrated with higher powers available in straight-forward extensions), and can be generated with very high repetition rates (100 MHz to 1 GHz) which lead to very high average powers."

Page from notes in my break-out session:

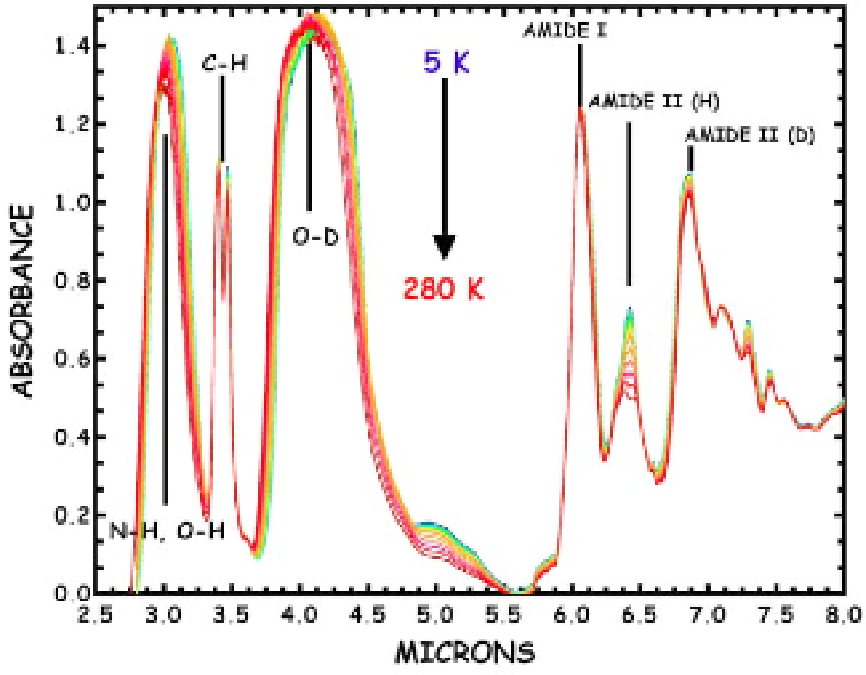
1) What do we need to say about user facilities?

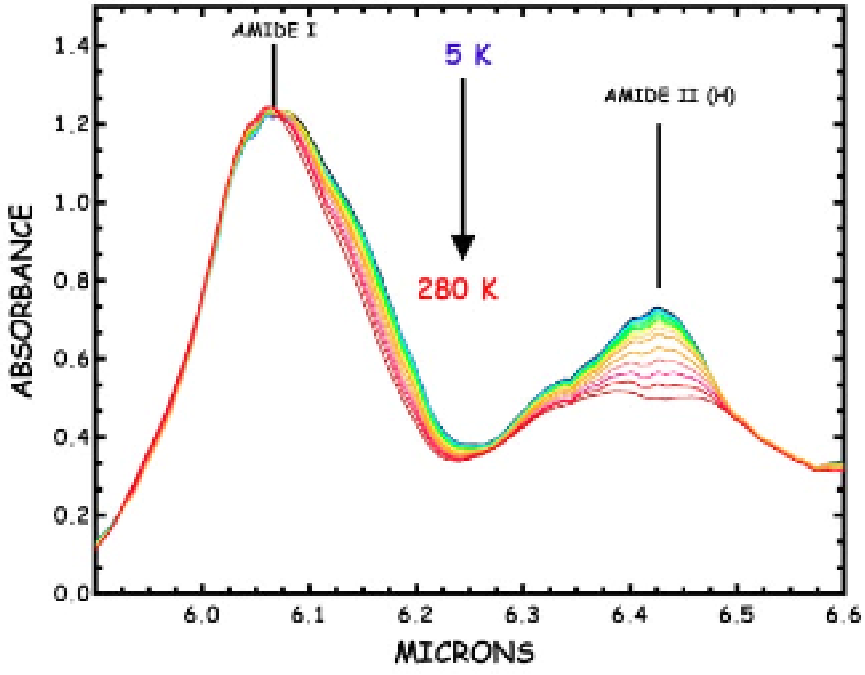
We want it all: high brightness, ultra-fast, ultra narrow, single pulse to kHz, multiple wavelengths from X-ray to FIR, high vacuum purged beam lines, spectrometers, etc.

Need a mix of a central facility and local focussed technology.

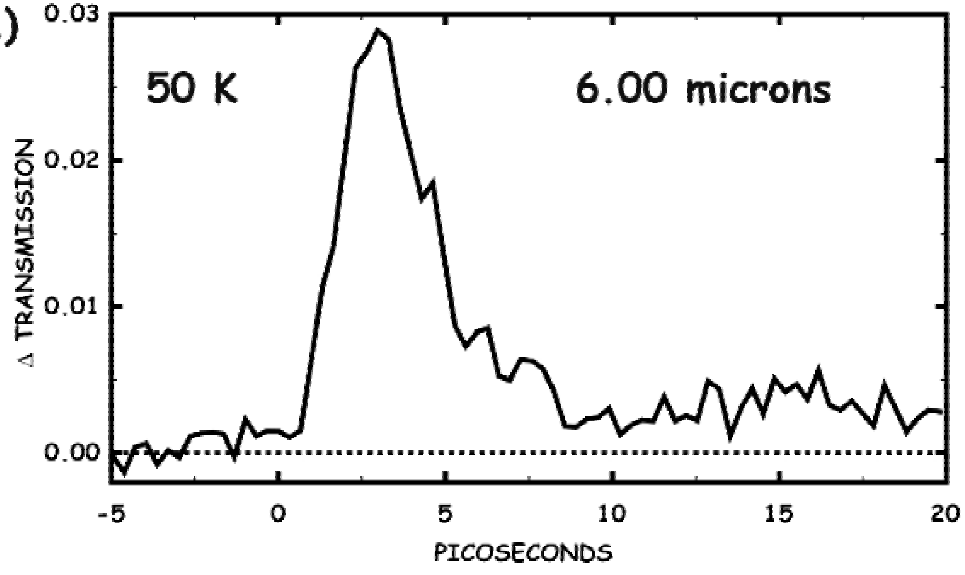
2) If you had an infinite amount of time/money, what experiment would you do?

HOLY GRAIL: Connect THz processes to biological

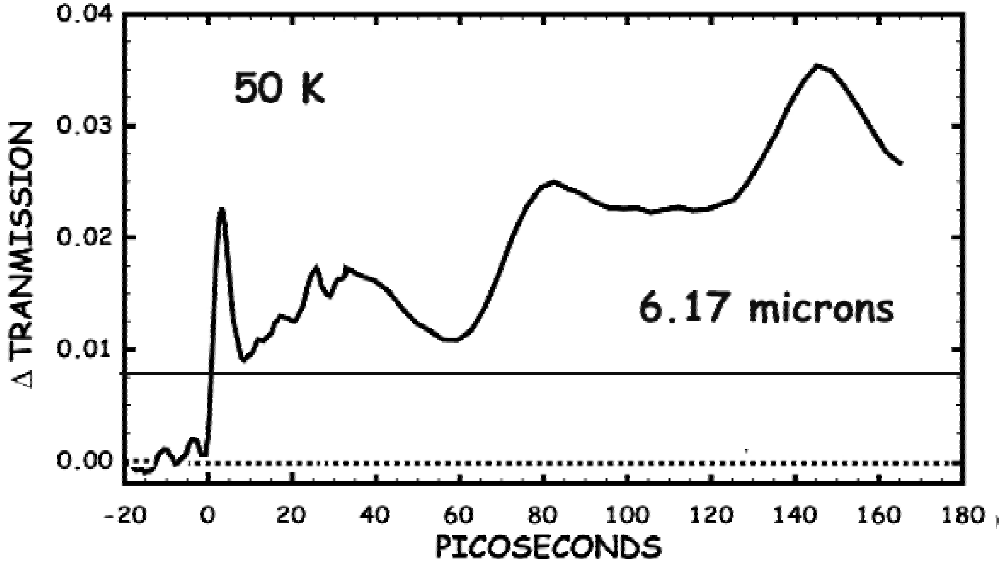

ABSORBANCE
MICRONS
C-H
O-D
N-H, O-H
AMIDE I
AMIDE II (H)
AMIDE II (D)
5 K
280 K


ABSORBANCE
MICRONS
AMIDE I
AMIDE II (H)
5 K
280 K

(A)


Δ TRANSMISSION
PICOSECONDS
50 K
6.00 microns

(B)


Δ TRANMISSION
PICOSECONDS
50 K
6.17 microns

In summary, I think this was quite a remarkable workshop which brought together for the first time a very diverse group of scientists, technology developers and funding agencies. Let's hope it catalyzes a real breakthrough in THz science, still very much a frontier area.