that stable transformation of crops with RNAi constructs results in stable modification of biochemical pathways which can result in improved productivity and quality of crops in the field.

Is the work on plant systems ignored in the award of Nobel Prize?

After the award of the 2006 Nobel Prize to Fire and Mello for the dicovery of the mechnism involved in RNAi, questions have also been raised arguing that recognition of the earlier work done on RNAi in plant systems was ignored. For instance, in a letter published in *Nature* on October 26, 2006, it has been argued that several aspects of the discovery that were cited in favour of the award including sequence specificity, RNA degradation and post-transcriptional nature of gene silencing were earlier demonstrated in plant systems, and were ignored during the award of Nobel Prize to Fire and Mello[9], since none of the scientists, who devoted themselves to RNAi work on plants shared the Nobel Prize.

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MEETING REPORT

Free-electron lasers and their applications*

The Indo-French workshop brought together accelerator physicists and users from the CLIO (Collaboration for an Infrared FEL at Orsay) Free-Electron Laser (FEL) in Orsay, France, accelerator physicists from the Compact Ultrafast Terahertz FEL (CUTE-FEL), and the latter's potential users in India. CLIO is an infrared FEL facility that has been operating for the last fifteen years at wavelengths from 3 to 100 μm. The CUTE-FEL is a terahertz FEL that is being built at the Raja Ramanna Centre for Advanced Technology. Ten scientists from France and twenty scientists and two students from India attended the workshop.

The workshop commenced with introductory remarks by Shiva Prasad, Director of IFCPAR, who welcomed the participants and briefed them on the objectives of the Centre. J.-M. Ortega then spoke on the CLIO FEL, emphasizing the unique features of the FEL – broadly tunable spectral range, appropriate pulse structure of picosecond pulses at MHz repetition rate, and high peak and average power (around 10 MW and 10 W respectively). He also pointed out the importance of value-addition to the facility by providing conventional lasers that are synchronized to the FEL pulses. S. Krishnagopal described the parameters of the CUTE-FEL being developed in India, and briefed the participants on the present status of activities. He emphasized the fact that a major part of the effort has been in the development of the technology of the linear accelerator and undulator that are part of the FEL. A standing-wave Plane Wave Transformer (PWT) linac has been developed, only the second in the world, and a 10 mA electron beam has been accelerated in this 21 cm long structure to 3.5 MeV, corresponding to an accelerating gradient of around 20 MV/m. A 5 cm period, 2.5 m long, planar undulator, using NdFeB magnets, has also been built and characterized. The remaining talks on the first day were devoted to further details of the two FELs. There were also talks from V. B. Asgekar on undulator development and Cherenkov FEL activities at Pune University, and from Ravi Kumar on FEL-related activities at the Institute for Plasma Research.

From the second day onwards discussions turned to applications of FELs. The French participants presented interesting work done on the CLIO FEL. They emphasized that for all of this work the CLIO FEL was a unique tool either because of the high power (enabling nonlinear studies), or the wide frequency tuning, or the convenient pulse structure.

C. Desfrançois discussed the structure of protonated peptides and drugs in the gas phase using the technique of infrared multi-photon dissociation (IRMPD) spectroscopy. He compared the IR spectrum of the biological peptide sequence RGD (arginineglycine–aspartic acid) with the one of a cyclic peptide containing the same RGD sequence (Arg–Gly–Asp–Phe–Val), and showed that the recognized RGD loop structure encountered in RGD-containing proteins is conserved in the gas-phase. He also showed the first gas-phase IR spectra of the very powerful

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anti-malaria drug artemisinin. Joël Lemaire elaborated on two different spectrometers that have been used at CLIO to perform IRMPD spectroscopy on trapped ions. The first is a lab-built transportable Fourier Transform Ion Cyclotron Resonance Mass Spectrometer. The second is based on a modified commercial radiofrequency ion trap, where ions formed from an electrospray ionization (ESI) source can be accumulated. The IRMPD spectra obtained for protonated nucleobases illustrated a case where different tautomeric structures are observed for the same species and where the predominant one corresponds to a non-classical structure.

A. Dazzi described a new method of infrared micro-spectroscopy. In this technique they use the photothermal expansion effect, detected by an atomic force microscope tip, probing the local transient deformation induced by an infrared pulsed laser tuned at a sample absorbing wavelength. This new tool ('AFMIR') opens the way of measuring and identifying spectroscopic contrasts not accessible by far-field or near-field optical methods and with a sub-wavelength lateral resolution.

J.-P. Galaup presented studies of carbon nanostructures such as fullerenes with a global approach. Their work demonstrates the versatility of the CLIO FEL through the study of the internal vibrational dynamic of fullerenes, followed by the synthesis of carbon nanostructures by laser pyrolysis. They have measured the population lifetime T_1 and the dephasing time T_2 of several active modes of the fullerene C_{60}. Because of the high symmetry of this molecule, only four modes are IR optically active. Here D. S. Misra pointed out that experimental conditions described were ideal for the growth of gem quality diamonds. C. Crépin showed that CLIO is a powerful tool to perform time-resolved experiments dedicated to vibrational dynamics, especially due to the large spectral range of CLIO. With very simple systems such as diatomic molecules (CO, DCl) embedded in van der Waals solids at low temperature, they have obtained the first observation of IR accumulated photon echoes.

A. Tadjeddine highlighted, through selected experimental results on the platinum–methanol system (relevant to fuel cells), the unique contribution of infrared-visible sum-frequency generation in understanding the influence of the structure of electrochemical interfaces on their reactivity. Knowledge of the structure of the very first layer in contact with the electrode surface is a key step for the comprehension of electrocatalysis processes that control the reaction. P. Boucaud reviewed the different properties of intersublevel transitions in quantum dots that can be probed with an FEL. Strong optical nonlinearities with large nonlinear susceptibilities can be observed for excitations in resonance with intersublevel transitions. Dynamic pump-probe spectroscopy in resonance with intersublevel absorption has provided the first evidence that the quantum dot relaxation is governed by polaron formation and the weight of the one-phonon component in the eigenstate. The precise knowledge of the quantum dot properties, obtained with CLIO, has led to a recent proposal to achieve optical gain infrared laser emission with self-assembled quantum dots.

The talks from the Indian participants also ranged over a wide spectrum of topics. S. Maiti examined the possibility of using FELs in the study of Alzheimer's disease. Ordered aggregation of physiological proteins into fibrillar structures has now emerged as a major cause of many age-related diseases. Modern laser-based techniques such as fluorescence correlation spectroscopy (FCS) allow us to resolve particle sizes down to sub-nanometer resolutions. The characteristic IR spectrum of the amyloid fibres, and the possibility of initiating aggregation by a light-induced pH jump, makes faster timescale kinetics potentially amenable to an IR-FEL.

K. C. Rustagi spoke about optical nonlinearities in nanostructures. Size and dimension dependence of optical nonlinearities has been of interest for a long time. There have been several reports of enhancement of nonlinearities due to the size dependence of intraband matrix elements even for nonresonant nonlinearities, both for semiconductor and metal nanoparticles, but few of them have stood careful scrutiny. He listed a number of important questions that could be addressed through experiments with an IR or terahertz FEL. R. Chari pointed out that excitons play a major role in the band-edge optical properties of semiconductors and exciton dynamics is an important area of study for device physics. Pump-probe spectroscopy using ultrafast lasers is especially suited to such work. She described experiments that used a combination of a femtosecond IR laser and a picosecond FEL to probe the evolution of the 1s-2p excitonic level absorption in a photoexcited semiconductor.

D. S. Misra gave an overview of the properties and applications of carbon nanotubes that have made them one of the most exciting new materials being studied today. He emphasized that they have excellent potential as electron emitters, and their field enhancement factor compares favourably with that of current emitters. He also presented details of the synthesis of carbon nanotubes in his laboratory. FELs could be used to synthesize nanoparticles in much larger quantities.

S. S. Prabhu enumerated the applications of terahertz spectroscopy in physics, chemistry, biology and imaging. He described their table-top terahertz setup that has been used for experiments on some chemically and biologically important molecules. He also discussed further experiments that would require high power, and could be performed with a terahertz FEL. S. Bhattacharjee talked about the generation of wideband terahertz radiation using a microfabricated folded waveguide Traveling Wave Tube (TWT) amplifier, and gave details of the fabrication of this device. He also briefly mentioned another approach to terahertz generation – using frequency upshift of an electromagnetic wave in an intense magneto-plasma medium.

S. K. Sarkar emphasized that the high power, wide tunability and quasi-CW operation of FELs make them suitable for applications in nuclear engineering. Potential areas of application include isotope separation and enrichment, reprocessing of spent fuel, and synthesis of new strategic materials. D. K. Palit explained that IR-FELs offer several advantages over conventional lasers for vibrational spectroscopy, because of rapid and continuous tunability over a wide spectral range (3–110 μm), capability of producing micropulses as short as 200 femtosecond and high peak power (as high as 50 μJ). Ultrafast vibrational spectroscopy has an advantage over electronic spectroscopy in revealing the microscopic details of the molecular dynamics.

In the midst of the user talks, there was, on the fourth day, a session devoted to short-wavelength FELs as fourth-generation light sources (4GLS). M.-E. Couprie summarized the global scenario. There are a number of 4GLS projects being proposed in the world – X-ray FELs in the US (LCLS), Europe (XFEL), Italy (FERMI), Japan (SCSS), Korea and China, as well as DUV-FELs in Germany (actually operational), France, UK, Italy and the US. She also gave details of the ARC-EN-CIEL project in France, which proposes an FEL down to around 1 nm. She summed up the deliberations of two meetings held in France focusing on the applications of such an FEL. These meetings have led to the development of a strong scientific case for a 4GLS in France, and some of the very impressive proposed applications were also discussed. R. V. Nandedkar gave an Indian perspective to fourth-generation sources, and pointed out that such a tool would revolutionize research in materials science, which has a very strong presence in India.

Towards the end of the workshop an evening session was organized on future FEL activities in India. Krishnagopal briefed the participants that there was already interest in India in a fourth-generation light source. Some discussions have already taken place with scientists at IISc, TIFR, etc., in this regard, and a presentation was also given to SAC-PM in August 2005.

The view that emerged from the discussions was that a tunable, femtosecond, high-power laser in the X-ray regime would be a dream-machine that would open up revolutionary applications in science. A. Tadjeddine pointed out that even a short-wavelength FEL going down into the water-window region (4 nm) would engender tremendous applications in materials science, nanotechnology, chemistry, biology, medicine, condensed matter physics, plasma science, etc. S. K. Sarkar emphasized that the high-current, high-energy, electron beam needed to drive such an FEL would itself have many useful applications in pulse radiolysis, neutron generation, plasma-based acceleration, etc., and would constitute a very important value-addition to any proposal.

The consensus was that a roadmap towards such an FEL, designed to deliver radiation in stages, should be developed immediately. At the same time, there needs to be wider deliberation within the user community on the advantages of a 4GLS to the Indian research community. The participants also cautioned that adequate attention needs to be paid to auxiliary facilities (conventional lasers, wet labs, diagnostic equipment, etc.) that will be needed by the users.

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RESEARCH NEWS

Crystal structure prediction – evolutionary or revolutionary crystallography?

S. L. Chaplot and K. R. Rao

It is a dream for material scientists to be able to predict the crystal structure of a material with given composition of elements under specific conditions of temperature and pressure. When this dream is realized it would be a boon in search for new materials of novel and exotic physical properties for a variety of applications. Recent work of Oganov and Glass[1] (Theoretical Mineral Physics Group of Eidgenössische Technische Hochschule [ETH] of Swiss Federal Institute of Technology, Zurich) seems to bring us close to achieving this dream. The group led by Oganov has been 'interested in the structure and properties of materials (mainly earth- and planet-forming materials) at high pressures and temperatures'. They perform theoretical studies using state-of-the-art *ab initio* simulation methods, 'ranging from atomistic to full quantum-mechanical, including such methods as *ab-initio* molecular dynamics and density-functional perturbation theory'

The ETH group has developed an evolutionary algorithm that enables random initial structures to evolve towards thermodynamically stable structures. They are able to reproduce known structures and predict new structures at high pressures in several elemental solids, for example, of oxygen, sulphur, carbon and nitrogen and of several molecular solids. The method requires calculation of free energy for any given structure. At present there are practical difficulties in calculating the free energy at high temperatures using *ab-initio* density-functional theory but this might be surmounted when more powerful computing resources become available. It is interesting to know how they carry out the evolutionary process. They start with a number (about 20 for a 10 atom unit cell) of randomly generated structures, given only the chemical composition of the material of interest, with no other experimental information; then they locally optimize and choose some of those structures with low free energies to create the next generation of structures through ideas like heredity, lattice mutation and permutation of atoms. Heredity involves matching slices of parent structures. The next-generation structure is obtained by combining the fractional coordinates of selected atoms from two parent structures. In lattice mutation the unit cell is strained randomly. Certain hard constraints, such as ensuring reasonable bond lengths are used to guide the evolution process. So the evolution is based on evaluation of energetically favourable structures (the lower the total energy content of the crystal, the more favourably it is stable); the cycle is repeated with the favourably chosen structures till the most stable structure is arrived at. The fittest would survive.

Purely from considerations of geometry and packing, billions of different structures are possible even for a modest crystal with 10 atoms per unit cell. Evolutionary