REGAE: New Source for Atomically Resolved Dynamics

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Motivation

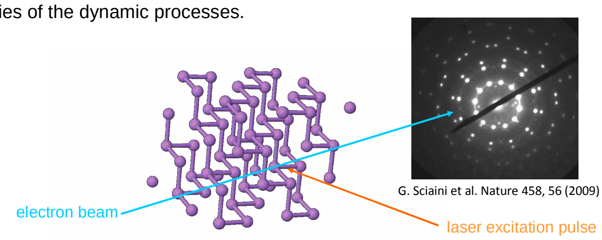
Electron accelerators were originally designed for studying nuclear reactions but nowadays they are beginning to be used in condensed matter and molecular physics, chemistry and biology for studying ultrafast dynamics of phase transitions and chemical reactions. Most of these facilities use either electron synchrotrons or free electron lasers to produce intense and short x-ray pulses to monitor and track the structural dynamics in the studied material. However, the size and the cost of 4th generation x-ray facilities (X-FELs) besides the less efficient interaction of photons with the sample but potential fast degradation of them make alternative light sources desirable.

An alternative is to use the electrons themselves. Time-resolved electron diffraction setups enable femtosecond temporal and atomic spatial resolution and with every electron detection this type of experiments will directly compete with the 4^{th} generation x-ray sources in many parameters. Here we present a new powerful tool that allows detecting structural dynamics in condensed matter on a femtosecond timescale – a relativistic electron gun for atomic exploration (REGAE). The relativistic energy of the electrons of about 5 MeV will make it possible to archive excellent temporal and spatial resolution necessary for making 'molecular movies'. Furthermore it will deal with one of the major problems for transmission studies. Where the sample thickness had to be on the order of 10 to 100 nm for lower energy electrons REGAE can cope with thicker samples up to 1 µm. This capability opens up the door to more complex structures such as proteins in the crystalline and liquid phase. The most important impact will likely be made in the fields of chemistry and biology where the central unifying concept of the transition state will come under direct observation.

Experiment

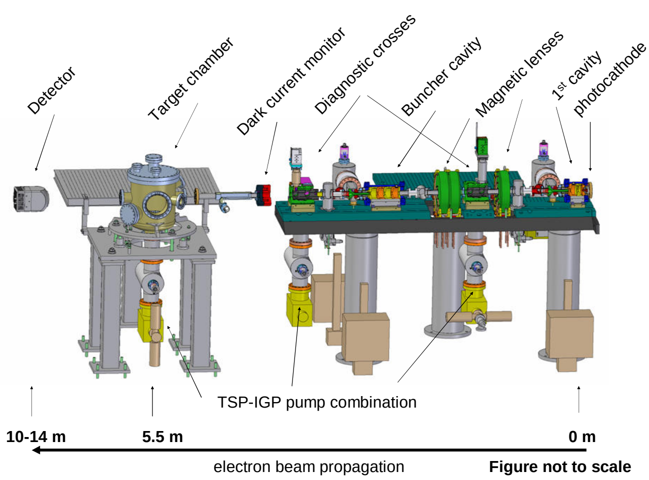
Pump-probe experiments

Pump-probe experiments are used for the detection of the temporal evolution of a specific aspect of the investigated system. The temporal propagation of the change in the investigated systems is triggered by a short excitation (pump) laser pulse and monitored with a short electron (probe) pulse. A controlled delay in between the probe and the pump pulse navigates through the single frames of stroboscopic movies of the dynamic processes.



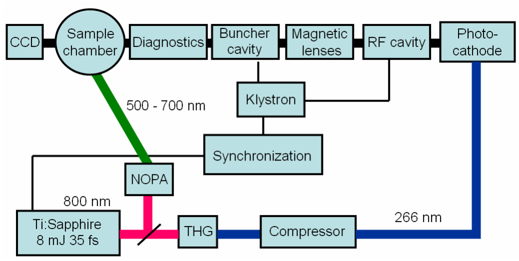
The electron probe pulse of REGAE (see below) can ultimately be made as short as 7 fs with a fundamental timing jitter of the entire system of 20 fs, limited by the electronics. This will allow resolving the dynamics of chemical reactions and phase transitions which usually occur on a 100 fs time scale or longer. A coherence length of 30 nm at the sample position provides access to a larger spatial resolution sufficient to resolve complex structures such as proteins and the energy of the electrons corresponds to an increased penetration depth.

The relativistic electron gun for atomic exploration REGAE



Femtosecond laser system and REGAE layout

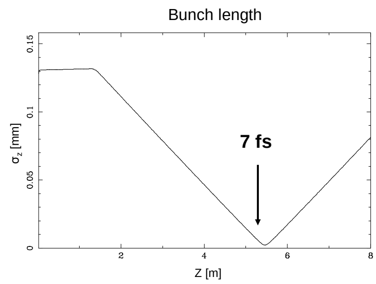
The femtosecond pump and photo excitation pulse is provided by a commercial Ti:Sapphire laser system. The third harmonic of the initial 800 nm from the laser is used to generate the initial electron bunch in the first cavity of REGAE and a nonlinear optical parametric amplification (NOPA) is used to prepare the pump pulse directed to the sample position.



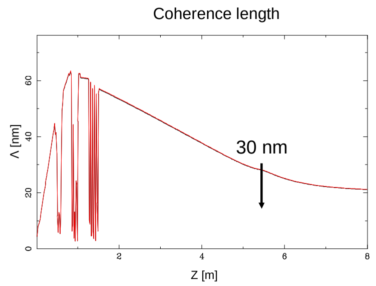
Preliminary results (Simulations)

ASTRA simulations

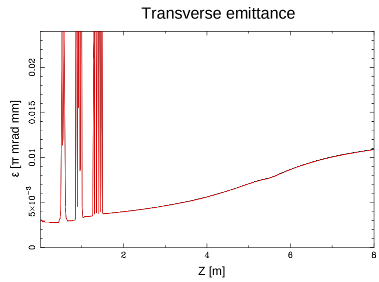
The program 'A Space Charge Tracking Algorithm' (ASTRA) was used to determine the optimum operational parameters of the REGAE. The simulation shows that the electron bunch length at the target position could be as short as 7 fs. This short pulse length provides unprecedented temporal resolution and is one of the most significant parameters of this machine.



The coherence length of a beam relates to the possible spatial resolution. The coherence length of the electron beam of REGAE is 30 nm at the sample position. With this it will be possible to resolve proteins in a solution or crystalline phase among other more complex structures.

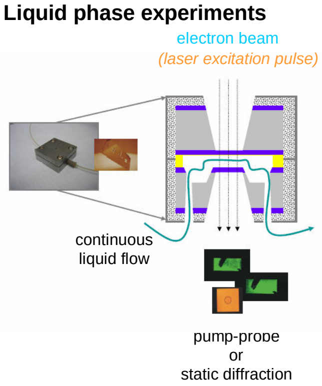


A small emittance allows smaller beam diameters, higher bunch charges and a shorter pulse length. It is also inherent in small diverging beams. The operational parameters of REGAE are set to operate with a tightly focused beam with a small transverse emittance.



Future experiments

Liquid phase experiments



Liquid phase samples can be studied if a solution film on the nanometer range can be created, confined and implemented into the harsh experimental conditions of the electron diffraction machinery. A special nano-fluidic sample cell has been designed, which will allow realization of this experiment within the REGAE setup. Controlling the flow of liquid solutions from the outside, static and time-resolved diffraction experiments can be thought of. Especially with the femtosecond temporal resolution of the REGAE machine, studies of chemical reactions, with the ability to structurally resolve their transition stages, will become possible.

Outlook

REGAE will be coming online around July 2011. Its design parameters open up the door to a new class of pump-probe experiments which cover a variety of dynamic processes from the solution phase to crystallized proteins. A comparable coherence length could only be achieved by the new generation of X-FEL light sources but REGAE will compete as a complementary tool with those billion dollar machines. With REGAE we are also closer than ever to shooting single-shot molecular movies. The actors are there, all we have to shout out now is: 'AND ACTION'!