Using coplanar wave guides to excite molecular motions in the frequency range of 10-1000GHz

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***Abstract*—We are presenting a new method to trigger molecular configurational chain reaction employing coplanar wave guides. This technique permits large field gradients at an individual molecule, direct electron transfer, and short excitation length down to the ps and sub-ps time scale. We present first results with excitation pulses of 1ns-100ps and compare these with simulations. Additionally we present simulations which show the feasibility of this technique up to the 1ps level.**

I. Introduction And Background

Structural changes of molecular systems triggered by electronic excitations play an important role in th functionality of biological systems, light-harvesting chemic systems and, last but not least, in the rational design synthetic structures mimicking biological systems whic convert chemical energy to motion. Pulsed X-ray sourc such as storage rings provide a new stroboscopic tool, often complementary to laser-based techniques, to probe not only the electronic excitations but also the structural response of molecules. We have recently demonstrated time dependent pump-probe X-ray scattering/diffraction capabilities with 100 ps time resolution[1].

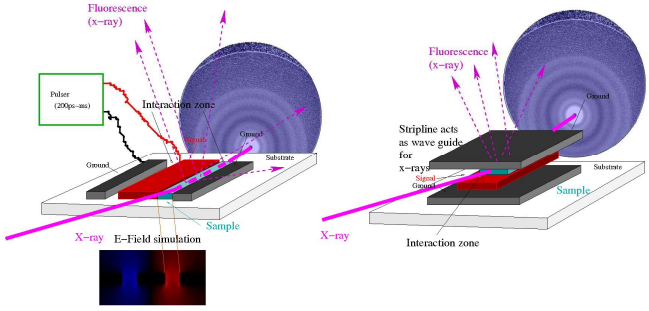

Figure 1: Usage of CPW sample cells for ultrafast x-ray scattering and spectroscopy experiments; the left panel shows a cell with horizontal alignment of the electric field (simulation of the electric field is shown in the inset), the right a cell with vertical alignment. The horizontal geometry will allow potential gradients of up to 0.5V over the dimension of one molecule with switching times in the order of 1ps. The vertical geometry will allow more complex structures modeling the materials properties in solar cells and organic light emitting devices.

A general problem of time dependent stroboscopic X-ray pump-probe experiments lies in synchronously triggering a molecular configurational chain reaction. In most cases, a laser excitation is used to trigger the reaction. Unfortunately, this excitation process itself is complex and typically requires multiple relaxation processes until the wanted reaction can take place. Often, creation of the electron-hole pair has a low efficiency resulting in high heatload on the sample, low excitation rates, and finally large sample damage. Excitation by electric fields or carrier transport is a much more efficient approach. Unfortunately, the fast switching requirements of this kind of experiments don't allow conventional setups. Our new approach addresses this problem by employing a strip-line device, e.g. coplanar wave guides (CPW), as sample cell, which is impedance-matched to a fast pulser or integrated optical switch.

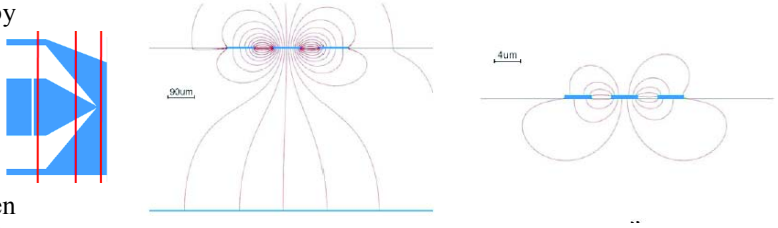

Figure 2: Simulation of the electric field in a tapered CPW; the left panel shows the device formed by an Austin switch combined with the taper and the transition in the micro CPW which is used as sample cell. The left and right red line indicates the position where a cross section of the electric field distribution is shown in the middle and right panel.

II. Results

The micro-wave pulse, produced by a power supply or an optical switch, is traveling along the length axis of a coplanar stripline, resulting in an electric field between the ground- and signal- electrodes. Due to the small dimensions, one can achieve large electric fields with low voltage pulses (1-5V). Including optical switches on the wafer, triggered by ultra-fast lasers, one can switch 500V in about 1ps. With a spacing of the electrodes of 1µm a field gradient of about 0.5V/nm can be achieved. Using the program package COMSOL we were able to provide a simulation of the electric properties. In Figure 2 a typical device and some representative simulation results are shown. The ohmic contribution of the impedance will be increased if the sample molecules are positioned in the gap between signal and ground electrode. Therefore, the electric field in presence of a micro-wave pulse will yield to a charge transfer in the sample material and between the electrodes. This effect will be frequency dependent so that the impedance will become frequency dependent and a part of the micro-wave power will be reflected. Dependent on the sample reaction, the peak shape will be deformed. In respect to the

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shortest possible pulses, this will be the ultimate limit. The small size of the structure results in multiple advantages. Besides the easy impedance adjustment to the source, a very thin sample thickness can be chosen. This is essential to ensure a complete or maximal excitation of the sample. By varying the gap size, the structure can be adjusted to the specific requirements of the sample material.

The combination of microwave characterization and x-ray probe provides large advantages. The microwave characterization permits to probe a large parameter space like frequency range, temperature dependence, or solvent dependence. Using loss spectroscopy will help to pre-select interesting sample conditions. The x-ray experiment will probe the sample under these conditions and visualize molecular motions with atomic resolution and cross correlate these with electronic excitations. Since the x-ray experiments are difficult and time consuming the pre-scanning of sample conditions are essential for the success of the experiment.

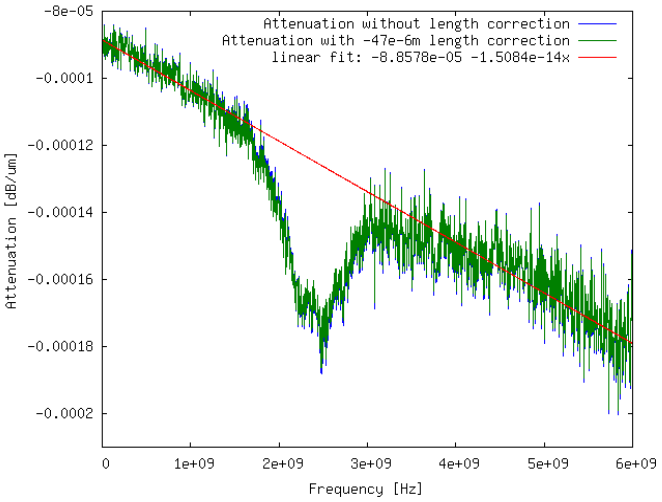

Figure 3: Attenuation/µm of a micro-CPW determined from absorption and reflection data of vector network analyzer in the frequency range of 3MHz-6GHz.

Our final goal is to develop loss spectroscopy up to the THz range. However, the time resolution of the existing x-ray experiment is in the order of 100ps. Therefore we started to develop the characterization with standard network analyzers in the 10GHz-range. Besides techniques based on continuous excitations we apply pulsed techniques to develop a loss spectroscopy which allows to determine even smallest amounts of materials. An example of these activities is given in Figure 3. The S-parameters of multiple micro CPW of different length but constant cross section were determined with a vector network analyzer. The power loss of each line for each frequency point is determined and a linear regression with the length of the line performed. The slope of this linear fit represents the attenuation per length unit. Taking dielectric loss into account one would expect a linear function with frequency indicated by the red line in Figure 3. The origin of the resonance like absorption around 2.5 GHz is presently unknown. We are investigating if a paramagnetic resonance of Cr_2O_3 may cause this effect. Between the conducting Au layer and the semiconductor substrate (GaAs) a Cr-layer ensures good mechanical contact between Au and the substrate. During the sputtering process this Cr-layer forms an oxide with the O on the surface of GaAs.

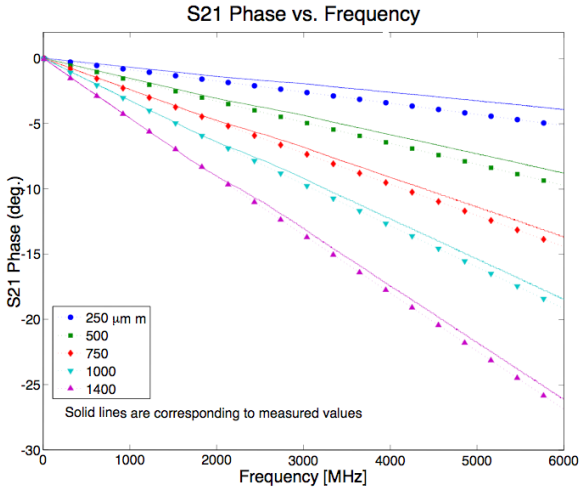

Figure 4: Simulation and measurement of the phase shift of various micro CPW in the frequency range between 3MHz-6GHz.

To optimize materials and geometry of the CPW simulations play an essential role. We presently use two different simulation packages (COMSOL and GENISIS). In **Figure 4** a comparison between simulations (GENISIS) and measured phase shifts of CPW with different length are shown. The good agreement between measurement and simulation demonstrates the reliability of simulation and measurement.

Based on these experiences in simulation and measurements we developed the first device, shown in Figure 5, which will allow to determine the frequency dependent transmitted power and phase of a 1ps pulse.

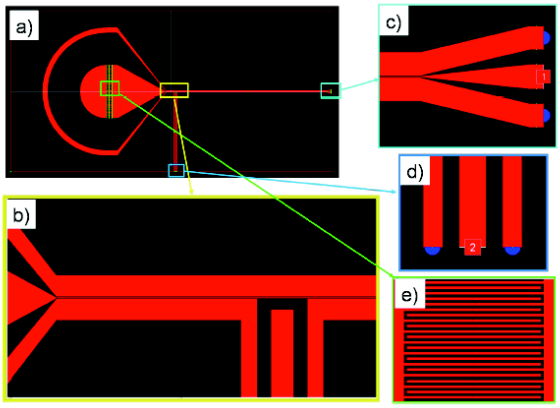

Figure 5: Device to measure power and phase of a 1ps pulse after passing a sample interaction zone.

REFERENCES

[1] Tiede, D.M., Zuo, X, Goshe, A,, Chen, L.X., Zhang, X., Attenkofer, K.,Beamline 11ID-D June 25 – July 4, 2006.