Investigation of the Dielectric Function of Guanine and Cytosine Heterostructures

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In recent year multilayered organic structures have attracted considerable attention[1]. Compared to bulk materials multilayered heterostructures can have unusual optical and physical properties which open new possibilities for optoelectronic devices.

It is well known that the guanine and cytosine rich DNA molecule can show p-type semiconducting properties[2]. In that case it is interesting to study the optical response of multilayer composed of very thin layers of guanine ($C_5H_5N_5O$) and cytosine ($C_4H_5N_3O$) molecules. Synchrotron radiation at BESSY II provides ideally suited means to investigate the optical properties of such DNA base heterostructures.

Bulk and thin multilayer films of guanine and cytosine on ZnO substrates were prepared by organic molecular molecular beam deposition under ultra high vacuum (10^{-9} mbar) conditions and measured *in situ* by means of Vacuum Ultra Violet (VUV) Spectroscopic Ellipsometry at BESSY. This measurement technique is based on the determination of polarization of light before and after reflection on the sample surface. The *in situ* measurements were performed at an angle of incidence of 68^0 in the range between 4 to 9.5 eV. For thickness determination and anisotropy evaluation supplemental measurements were carried out in the transparent spectral range below 4 eV at different incidence angles.

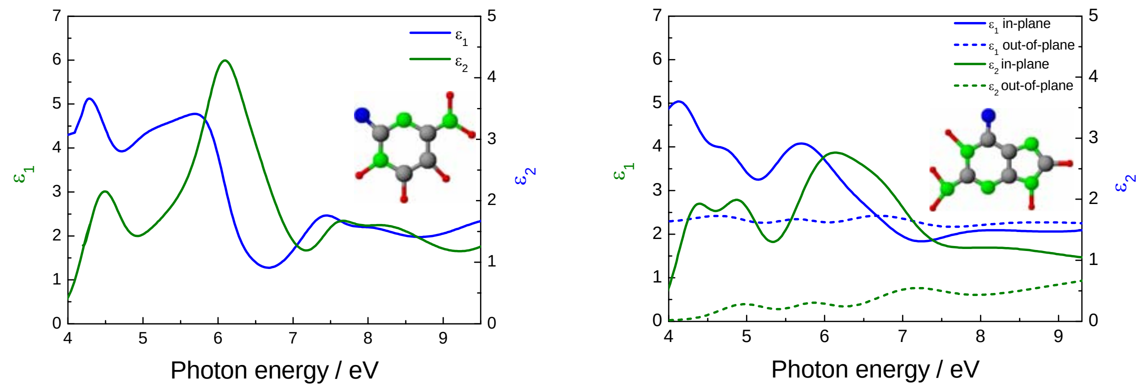

Figure 1: Dielectric functions and molecular structure of cytosine (left) and guanine (right).

Good agreement between the measured and simulated data was achieved using an isotropic model for cytosine and uniaxial anisotropic model for guanine. In Fig. 1 the resulting dielectric functions of thick bulk-like cytosine and guanine films are presented. These dielectric functions are used to simulate thin multilayer of these molecules.

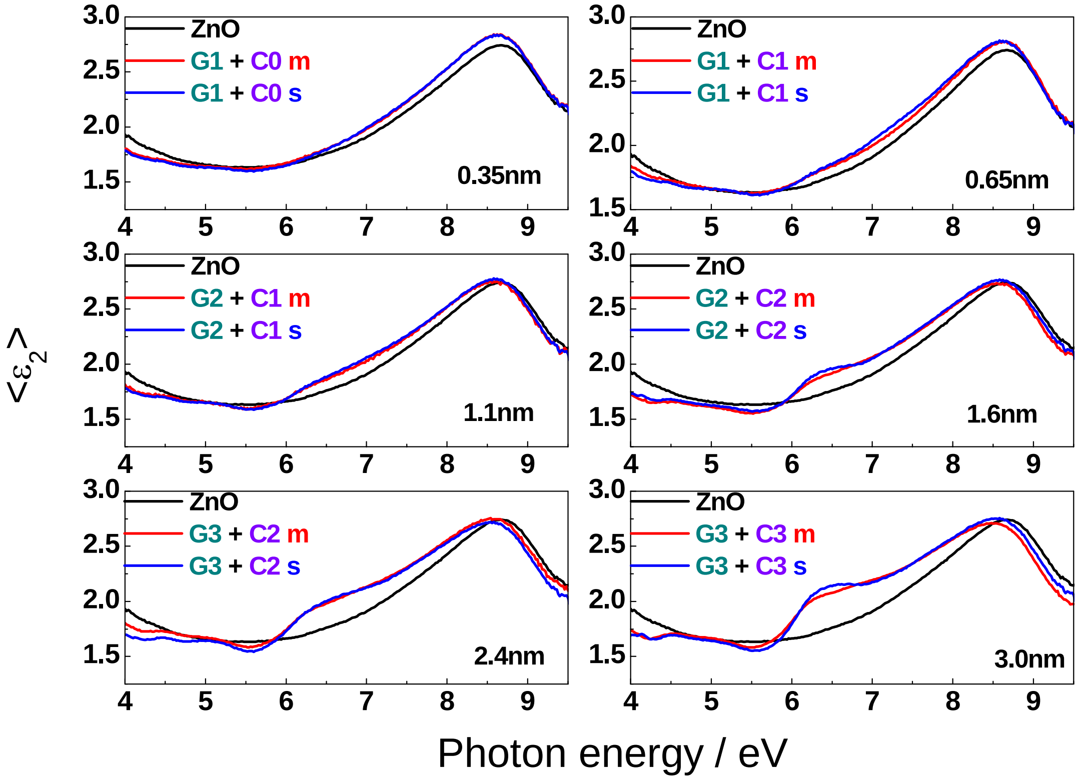

Figure 2: Measured (red) and simulated (blue) effective dielectric function for the multilayer structure and the clean substrate (black) for comparison. G2+C1 in the legend means that the effective dielectric function is measured after depositing the second guanine layer (G2) on the first guanine (G1) + cytosine (C1) layer stack.

Figure 2 shows the measured and simulated effective dielectric function of multilayer structures starting from guanine together with the effective dielectric function of the bare substrate. Three alternative layers of guanine and cytosine are grown on the ZnO substrate. From the determined thickness of the cytosine and guanine in the multilayer, we have a single layer of each to start with and have two layers after the first two depositions[3,4]. As observed, even for the first thin layer there is considerable change in the effective dielectric function indicating the strong optical absorption of these DNA bases. The multilayer is modelled with sharp interfaces and the determined thickness is as expected suggesting a highly ordered multilayer structure. The slight deviation in the simulated spectra occurs because the cytosine layer is considered as isotropic as in the bulk films. However, in the ultra thin layers on silicon cytosine exhibits anisotropic behaviour[3].

Layers	Peak position in the effective dielectric function / eV					
Cytosine Bulk Thin Film	- -	4.44 4.50	5.10 -	6.05 6.42	7.50 -	8.10 -
Guanine Bulk Thin Film	4.35 4.46	4.88 5.06	5.80 -	6.40 6.92	7.90 -	8.80 -
Multilayer	4.52	5.05	-	6.32	-	-

The peak positions present in the ultra thin multilayer are observed to be shifted to higher

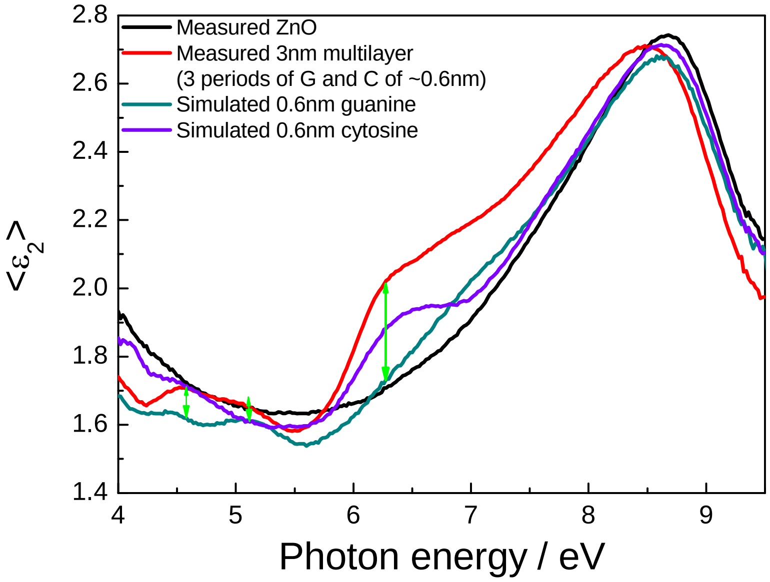

Figure 3: Compared <ε_2> of 3nm thick multilayer with simulated thin guanine and cytosine layer

energy. From figure 3 it is observed that the peak around 6.2 eV is strongly attributed by the cytosine layer while that between 4 eV to 5.4 eV stems more from the guanine layer.

The results presented are a good starting point for a more detailed understanding of the arrangement of molecules in the multilayers and their interaction. Further measurements are planned starting with a cytosine layer. The evaluation of first monolayer spectra will give insight in the interaction of molecules with the substrate.

Acknowledgement:

The author would like to acknowledge the BMBF projects 05 KS4KTB/3 and 05 ES3XBA/5, IRTG "Materials and Concepts for Advanced Interconnects" and the DFG Collaborative Research Center 379 "Arrays of Micromechanical Sensors and Actuators".

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