VUV-SE spectra of guanine layers on H-Si(111) surfaces

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Among DNA bases (adenine-A, thymine-T, guanine-G, cytosine-C), guanine (Figure 1) is important in the field of bioelectronic devices at molecular scale like biomolecular nanowires [1,2]. In order to identify the electronic transitions and determine the optical constants (**n**, **k**) of the guanine layers deposited on H-passivated Si(111), vacuum ultraviolet (VUV) spectroscopic ellipsometry (SE) technique is employed. A literature survey did not reveal any investigation concerning the optical constants of any DNA bases. Guanine layers with different thicknesses namely ~40 nm and ~100 nm were grown on H-Si(111) surfaces by organic molecular beam deposition (OMBD) under ultra-high vacuum (UHV) conditions (base pressure ~ $3 \cdot 10^{-9}$ mbar). Prior to guanine deposition, clean H-Si(111) surfaces were wet-chemically prepared as follows: first the substrates were degreased of organic contaminants by rinsing in isopropanol and de-ionized water; afterwards the native oxide was removed by etching for 2 min in hydrofluoric acid (HF 40%) resulting in H-terminated Si(111) surfaces showing a sharp 1x1 LEED pattern. Guanine was evaporated onto H-Si(111) surfaces with a rate of 2nm/min from a Knudsen cell at a temperature of about 510K. During the guanine deposition the substrates were kept at room temperature (RT).
The VUV-SE measurements were performed on the guanine layers with the VUV ellipsometer operating with the **3m**-**N**ormal-**I**ncidence-**M**onochromator **1** as light source and MgF_2 Rochon prisms as polarizer and analyzer. The SE spectra were recorded in the photon energy range from 3.0 to 9.5 eV at an angle of incidence of 68°. To our knowledge, these are the first SE measurements of guanine layers on H-Si(111) surfaces prepared under UHV conditions using synchrotron radiation. Unlike the aging processes of guanine layers on LiF substrates observed under high-vacuum conditions [3], no aging of the guanine layers was observed after 2 days in UHV at a pressure of 7×10^{-10} mbar. The exposure to the synchrotron radiation did not cause any deterioration of the samples.

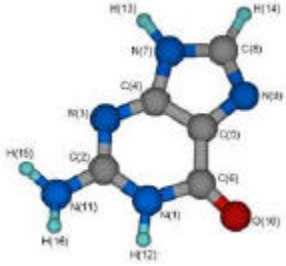

Figure 1. Chemical structure of a guanine molecule.

Figure 2 shows the real $<\varepsilon_1>$ and imaginary part $<\varepsilon_2>$ of the measured effective dielectric functions of guanine layers on H-Si(111) surfaces. Measurements performed as a function of azimuthal angle showed that the guanine layers are optically isotropic. The spectra are dominated by strong interference features at 3.9 eV in the thin layer and 3.97 eV in the thicker one. Above 4 eV, the spectra are dominated by the features due to guanine involving electronic transitions with π-π^* character. Three features can be distinguished in the spectra of both guanine layers. The first peak corresponds to the HOMO-LUMO transition. The positions of the features for 100 nm layer thickness are at 4.77, 5.41, 6.11 eV and a shoulder at 6.76 eV. All features are shifted towards higher energy for a layer thickness of 40 nm. Absorption spectra of high-vacuum deposited guanine layers on LiF substrates exhibit features at lower energy values (4.31, 4.90, 6.20 and 6.70 eV) compared to the energy positions in SE spectra. The shifts in peak positions may be related to a difference in the thickness of guanine layers. However, further experimental and theoretical investigations are required. A theoretical study involving the calculations of electronic transitions of guanine molecule and dimers using DFT theory at different levels is in progress.

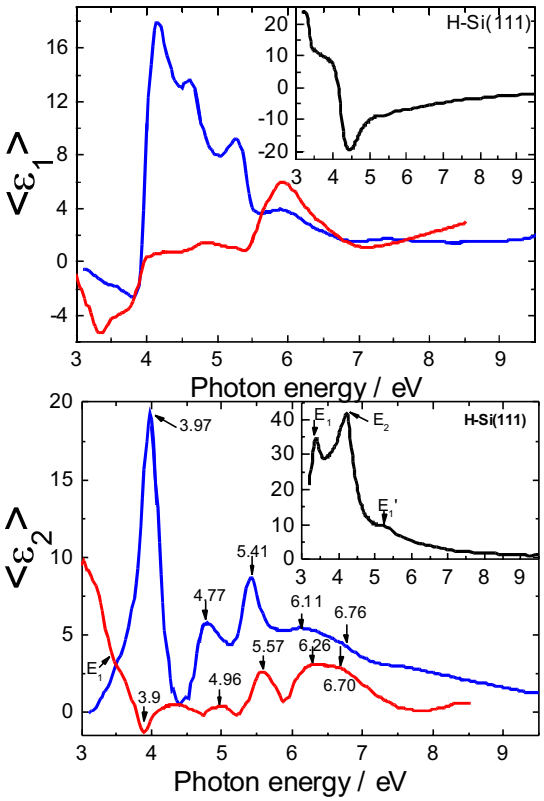

Figure 2. Measured effective dielectric functions $<\varepsilon_1>$, $<\varepsilon_2>$ of guanine layers (~ 40 nm – red lines; ~ 100 nm – **blue lines**) on H-Si(111). In the inset $<\varepsilon_1>$, $<\varepsilon_2>$ of the H-Si(111) substrate are shown.

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[1] A. Calzolari, R. Di Felice, E. Molinari and A. Garbesi, "Appl. Phys. Lett." 80 (2002) 3331

[2] R. Di Felice, A. Calzolari, E. Molinari and A. Garbesi, "Phys. Rev. B", 65 (2002) 045104

[3] T. Yamada and H. Fukutome, "Biopolymers", 6 (1968) 43-54