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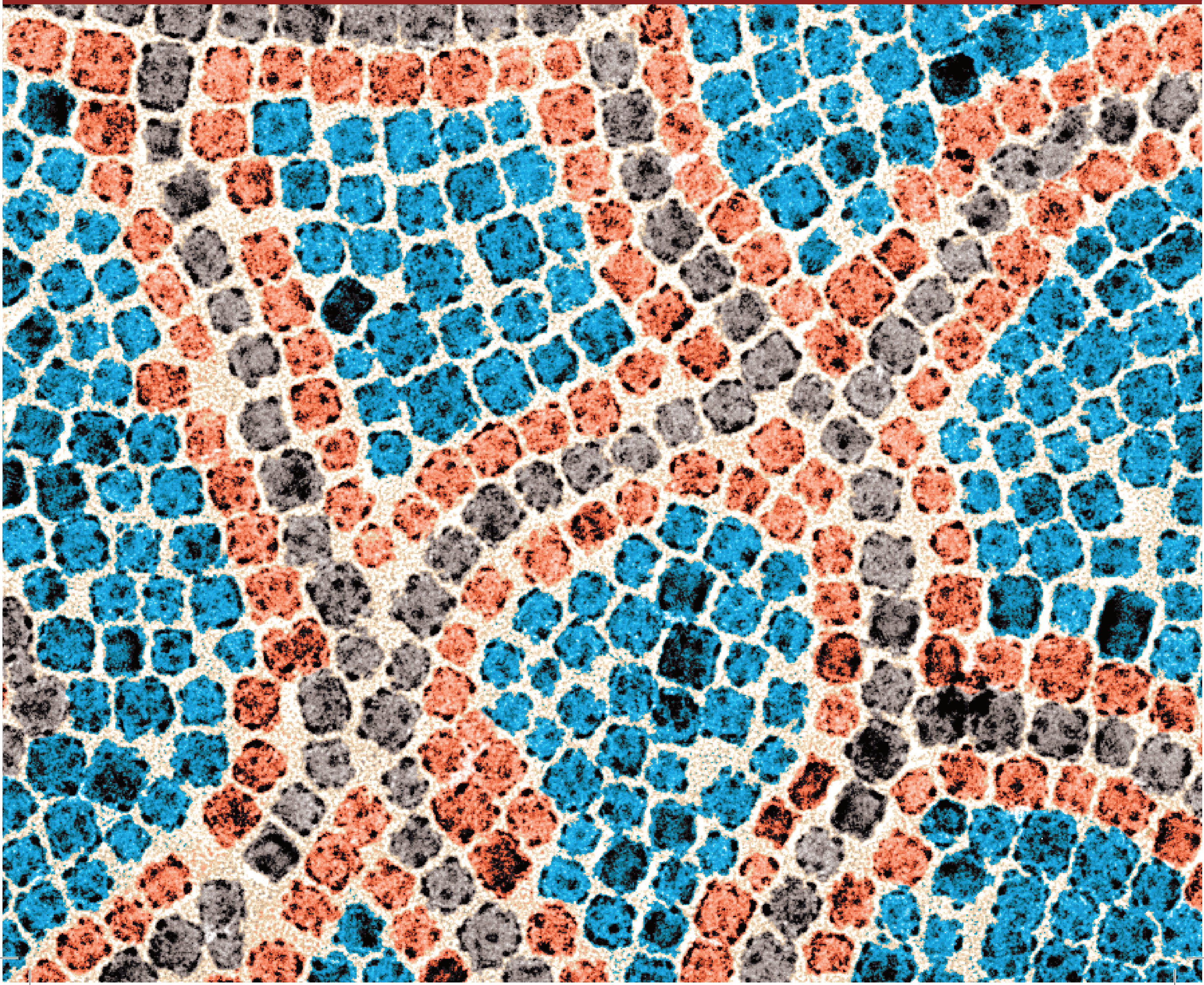
ABSTRACTS



Oral Presentation **O17-5**

QM/MM Simulations of the Immobilization of Isolated Proteins on Graphite Surfaces via Gold Atomic Clusters

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The stable immobilization of proteins on surfaces is a key issue for a new generation of bioelectronic devices [Trends Biotechnol. 19 222 (2001)]. Such applications require that proteins be oriented in a way that their active sites are free to bind other molecules. In the past, different gold surfaces have been investigated as protein supports, since it was discovered that proteins with free cysteines can form strong gold-sulfide bonds. However, proteins deposited on gold surfaces tend to form monolayers, and thus large areas within the proteins are hidden. We have succeeded in immobilizing isolated proteins on a graphite surface decorated with size-selected gold clusters deposited from a cluster-beam source [Nature Materials 2 443, (2003)]. This approach is now being exploited in the development of a novel biochip for protein screening by a spin-off company. Nonetheless, many fundamental questions remain. Experimentally, there are several challenges to examine the structure of the immobilized proteins; X-ray-diffraction microscopes cannot be employed since the proteins are isolated, while STM distorts the protein structure. On the other hand, modeling can provide an attractive approach to obtain an idea of the structure and binding of an isolated protein immobilized on a surface. In our theoretical group, we employ a QM-MM approach developed by us [J. Phys. Chem. B 107, 13728 (2003)] that combines the SIESTA methodology (DFT approach) with an empirical force field. In this talk, we address the nature of the interaction between a human oncostatin M (OSM) molecule and an Au75 cluster pinned on a graphite surface. For instance, we show that the cysteine residues of OSM can form strong bonds with the surface atoms of the gold cluster. The orientation and structure of the adsorbed protein is analyzed. QM/MM results are compared with experimental data.

Oral Presentation **O17-6**

Arbitrary Polymeric Nanodevice for Single-Cell Analysis

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Experiments on a bulk cell population in a petri dish provides averaged data from which single cell behavior is difficult to be detected and extracted. Distinguishing this individual difference would be important to pharmacists and biologists. Therefore, single-cell analysis (SCA) has been listed as one of the "10 Emerging Technologies" by Technology Review.

The critical step in analyzing single cells is to anchor the cells in situ. We have developed a three-dimensional lithography system that allows fabrication of a submicron polymeric device on a normal cell culture plate, to separate and trap single cells mechanically. No additional photonic, electric field or mineral oil is required, unlike the conventional SCA manipulating tools, such as laser tweezers, dielectrophoresis or microfluidic droplet array. The material used is non-immunogenic and compatible with the process of single-cell RT-PCR and sequencing.

Arbitrary three-dimensional devices can be fabricated and scanned layer-by-layer through a two-photon absorption (TPA) process with a resolution of up to 300 nm. Fully automatic array function provides higher throughput from computer design to chip output. The total scanning area is scalable, up to an area of 10 cm x 10 cm. With these features, a device of a dimension of 120 μm has been designed to trap one to seven hepatocytes for single cell analysis, with the additional benefit of observing cell-cell interaction in a single experiment.

Polymer-based devices provide a cell friendly platform with minimum residual metallic or semiconductor material that may compromise the cell culture. Three-dimensional lithography further offers the ability to mimic the microcellular environment, maintaining cellular function better than the conventional two-dimensional platform.

Oral Presentation **O17-7**

Simulation and Fabrication of a Mechano-Optical Sensor for Nano-Displacements

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We present the simulation and fabrication of a novel and highly sensitive mechano-optical sensor for nano-displacements, based on microcantilevers suspended above a Si_3N_4 grated waveguide (GWG). The presence of a dielectric object, in this case a suspended cantilever, in the evanescent field region of the GWG may lead to the occurrence of propagating modes for wavelengths inside the stop band of the grating, and so to resonances (defect modes) inside the stop band.

The 2D bidirectional eigenmode propagation (BEP) method has been applied to analyze the effect of cantilever displacement on the optical transmission spectrum of the GWG. The simulation results show that as the cantilever approaches the grating, the first near band-edge resonance peak is pulled inside the stop band and its spectral width decreases. The resolution of displacement measurement is estimated to be 0.2 nm for a 200 nm thick cantilever at a 200 nm initial gap, assuming a signal-to-noise ratio (SNR) of 20 dB.

Integrated microcantilever-GWG devices have been fabricated successfully using MEMS techniques. Uniform gratings have been defined with laser interference lithography. SiO_2 cantilevers with low initial bending (i.e., low stress) have been fabricated by combining the tetra-ethyl-ortho-silicate chemical vapor deposition (TEOS-CVD) and plasma-enhanced chemical vapor deposition (PE-CVD) oxides, and by releasing them using a tetramethylammonium hydroxide (TMAH) wet-etching solution, followed by a freeze-drying process. High-resolution-SEM and AFM measurements revealed that the initial bending of 30 μm long cantilevers is as low as 250 nm. Additionally it was found that TMAH etching improved the quality of the waveguides by reducing surface roughness from 1.41 nm down to 0.46 nm. The measured stop band of the GWG agrees well with the calculated result.

The simulation, successful fabrication, and initial optical characterization results demonstrate the potential of the integrated microcantilever-GWG as a novel and compact mechano-optical sensor for nano-displacements.

Oral Presentation **O17-8**

Electrochromic Nanoparticle Ink: Displays and Color-Switchable Glasses Fabricated by Liquid Processes

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Color-switchable devices, such as displays and color-switchable glasses, have been fabricated by means of the "*electrochromic nanoparticle ink*" by liquid processes.

For the electrochromic ink, we have developed the new method to synthesize the nanoparticles of Prussian blue (PB) and its analogues. With our synthesis, dense "ink" of the PB nanoparticles, e.g. 0.1g/ml, can be obtained. Consequently, various conventional coating and printing methods can be used in high-quality micro-fabrication. In addition, multi-color device is possible by means of the PB analogs having various colors.

The electrochromism of the PB nanoparticle films fabricated by spin-coating on a transparent conducting oxide (TCO) was observed; the color changes between blue and transparent reversibly by applying voltage. The electrical color-switchable glass with electrolyte sealed between opposed two TCOs with was fabricated, exhibiting electrochromism only with a 1.5 V dry battery even after operations of 10^5 times.

Various patterns of the nanoparticle thin film can be also printed on substrates using photolithography or inkjet printing techniques. For example, we have developed a display device switchable between different two patterns electrically. This device exhibits very fast response, less than 200 ms.

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