Nanocrystalline Diamond Thin Films for MEMS and Biomedical Devices

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The main aim of the NIRT project is to synthesize, characterize and model the nanocrystalline diamond thin films to utilize its extraordinary properties in various applications such as biomedical devices, MEMS structures and RF-MEMS devices. The research focus is in the following areas:

(i) Synthesis and Processing of Nanocrystalline Diamond Films by Microwave Plasma Enhanced CVD:

The primary objective of this project is to synthesize and characterize the nanocrystalline diamond (NCD) films for building the microelectromechanical systems (MEMS) and biomedical devices as they allow designing the complex mechanical elements with micrometer feature sizes by tailored material properties at the nanoscale to achieve the highest performance. The NCD films were deposited by microwave plasma enhanced chemical vapor deposition (MPECVD) in CH_4, Ar, and H_2 gas phase system at temperatures ~ 700- 750°C and pressures in the order of 90-120 Torr. Integration of dissimilar materials is required to realize more applications but it involves various challenges due to the fundamental differences in the properties of dissimilar materials. In regard to this, an initial effort has been successfully demonstrated to integrate the metal oxide nanowires of ZnO with NCD films. ZnO possess good electrical, optical and piezoelectric properties, hence the synthesis of new class of composite material if exploited fully might have extraordinary properties. The preliminary studies have shown that the nanowires and the grains of the NCD are well intercalated (see Fig.1. (a),(b),(c)).

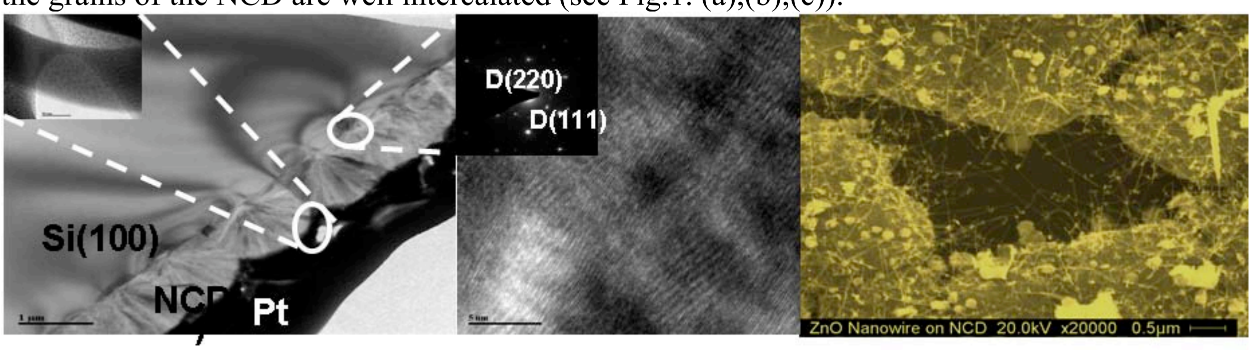

Fig.1(a) Fig.1(b) Fig.1(c)

(ii) Nanoscale Modeling of the Growth of Nanocrystalline Diamond Films

The study is aimed at performing an atomistic molecular dynamics (MD) simulation of nanodiamond using classical interatomic potentials to investigate its mechanical and tribological properties. The quality of interatomic potentials becomes a critical issue for realistic MD simulations. An analytic Bond Order Potentials (BOP's) has been developed for carbon and hydrocarbons that are based on many-atom expansion for the bond order within the tight-binding representation for the electronic structure. The breakthrough was achieved in the ability to model accurately the process of breaking and re-making of bonds. The construction of analytic BOP's for nanodiamond proceeded through 3 steps. An extensive first-principles density functional simulations was performed on various diamond crystalline phases including linear chain, square, graphite, diamond, simple cubic, fcc, and bcc structures that describe one, two and three dimensional coordinations of carbon atoms in solid state environment. Large-scale simulations

were performed on both atomic and electronic structure and created an extensive first-principles database with binding energies, elastic properties and band structures as a function of interatomic distances. The second stage included fitting the first-principles database by two-center orthogonal tight-binding model for electronic structure. Large amount of first principles data was described by fitting tight-binding hopping integrals as a function of interatomic distance. The environment dependence is the key in describing various low-coordinated structures including the surfaces of the nanodiamond grains. Therefore, the modification of two-center tight-binding model was performed to include the environment-dependent hopping integrals in BOP theory.
It was realized that precision machining and nanoscale fabrication of nanodiamond based MEMS and biomedical devices requires an investigation of high-pressure behavior of diamond including contact-induced phase transformations and anomalous elastic-plastic behavior. The prime goal was to investigate the high-pressure induced plasticity in relation to the nanoscale manufacturing process of nanodiamond devices. It was found that the shear stresses are the driving forces for the creation of both point and extended defects in nanocrystals subjected to mechanical load. We performed the density functional calculations of shear stresses in diamond subjected to uniaxial compression along three low-index crystallographic directions, <100>, <110>, <111> (see Fig. 3). It was discovered that the shear stresses exhibit non-monotonic behavior, see Fig. 2. This important result provides key information for understanding the dynamics of plastic deformations. In particular, the non-monotonic dependence of shear stresses on uniaxial compression might result in a significant delay or even freezing of the plastic deformations during mechanical load of NCD based devices.

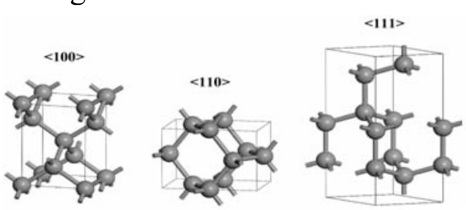

Fig.2

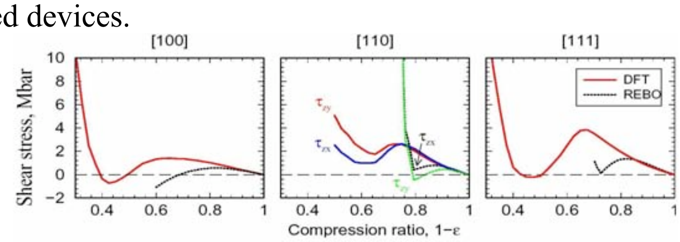

Fig.3

(iii) Nanocrystalline Diamond for Biomedical Applications

(a) NCD films for glucose detection: With its unusual chemical, physical, electrical and biocompatible properties, NCD has attracted much attention due to the need of a robust and stable bio interface for implantable biosensors to operate even in harsh environments. In our study, a glucose sensor has been successfully fabricated on a modified nitrogen-doped nanocrystalline diamond (NCD) electrode (see Fig. 4).

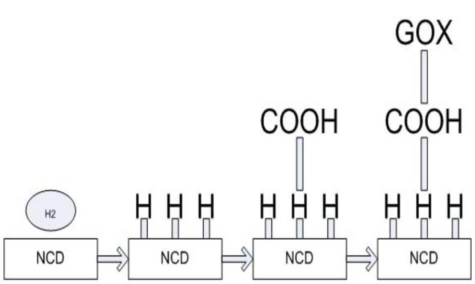

Fig. 4

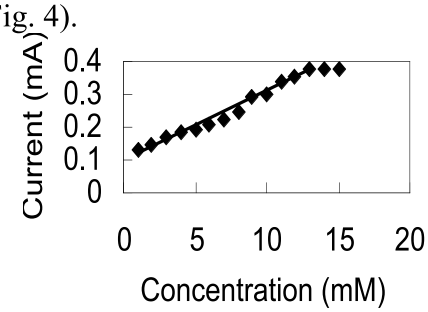

Fig.5

A hydrogenated surface was obtained on NCD films by exposing them to hydrogen plasma. The NCD electrode was functionalized by Carboxyl functional groups and the glucose oxidase (GOX) enzyme was immobilized. Cyclic voltammograms (CV) were performed to evaluate the response of the NCD electrode with different glucose concentrations. A linear calibration curve of glucose sensing has been obtained over the concentration range up to 13 mM in a phosphate buffer, as shown in Fig. 5.

(b) Nanocrystalline Diamond based micro fluidic lab-on-a-chip: Nanocrystalline diamond has attractive properties for use as a base material in microfluidic devices. Its chemical inertness, UV transparency, and high thermal conductivity make it suitable for incorporation with both active and passive devices, such as channels, mixers, reaction chambers, pumps, heaters, and sensors for measuring temperature, flow, impedance, pH, etc [1]. However its biocompatibility has not been fully exploited for biological lab-on-a-chip devices. Nanocrystalline diamond's inertness coupled with its surface smoothness can lead to it being an excellent material for devices handling proteins, DNA's, cells etc. NCD is a highly hydrophobic material, but its hydrophobicity can be controlled by post-deposition processes [2]. This research is exploring the use of diamond coated chambers for Chromatin Immuonoprecipitation-on-a-chip device. In the CHiP process, the sample is rinsed after each step to remove waste and retain the DNA of interest which is later subjected to PCR. This necessitates that the chambers be built with materials that exhibit minimal non-specific binding. The use of NCD can result in samples with higher purity as compared to the conventional materials with less stringent wash protocols, making the whole process faster and easier.

The immediate goal of this project is to analyze the biomolecular binding to NCD as compared to silicon and silicon dioxide. Towards this goal, the binding tests were performed by cross linking fluorescent DNA on various substrates using Formaldehyde for different time durations. The samples were washed using different wash cycles in the CHiP process. The substrates were then washed and inspected in a fluorescent microscope. The quantitative results are graphically illustrated in Fig. 6. The graph shows relative peak intensity of phosphorescence due to residual DNA. The data confirms that the DNA molecules bind least to NCD in nearly all instances. The next step will be to compare diamond with polymers, both epoxies and resins.

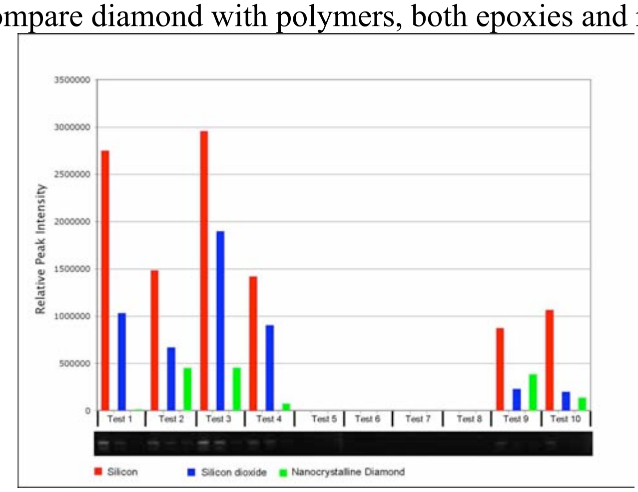

Fig. 6: DNA binding on different materials. Smaller peak intensity depicts lesser degree of binding

(iv) Nanocrystalline Diamond for RF/Microwave MEMS

NCD RF-MEMS (micro electro mechanical systems) have the potential to advance the capability and reliability of many types of microwave systems. Such devices could play an important role in revolutionary wireless base-station architectures that move power amplifiers from ground-level, air-conditioned buildings to the top of the antenna tower for direct integration with smart antenna arrays – eliminating 50% cable-induced power loss that plagues current base-station designs. Microwave sensors and communication systems that will be ubiquitous in future battle-field environments can become smaller and lighter, and able to operate under more extreme conditions. High-power space-based platforms can also benefit from improved thermal performance, extending operating lifetime and therefore lowering cost. These advances are possible because NCD RF-MEMS switches and tuning elements have the same advantages as conventional RF-MEMS devices (very low loss and DC power consumption, high linearity and isolation) but can handle much greater power (in the kW range) and operate at extreme temperatures (850°C, Kohn 2003[3]). These characteristics make them compatible for direct integration with high-power transistor technologies such as SiC and GaN.

The objective of this project is to develop a series of NCD RF-MEMS devices leading to an advanced technology for microwave phased-array antenna distribution networks. The first topologies being investigated are integrated, thin-film NCD-on-silicon high-power terminations. Architectures for switches and tuning elements will then be developed to produce phase- and amplitude-controlled networks. Efforts to integrate NCD based devices with thin-film ferroelectrics, to realize highly-functional phased-array elements with very wide electronic-tuning capability, are also underway. The research methods include numerical (electromagnetic, mechanical and thermal) modeling, thin-film fabrication and characterization.

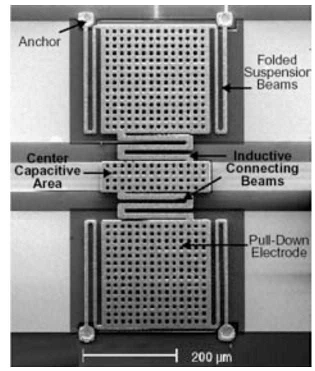

Figure 7 - RF MEMS switch (Pacheco, 2000) [4].

The University of South Florida has established several important external collaborations as part of this effort. A graduate student exchange is being planned for early 2006 with Dr. Erhard Kohn at the University of Ulm (Germany), a world-renowned expert in thin-film diamond growth and applications. We are also working closely with research scientists at Raytheon in order to shape the development of the RF devices in ways that will facilitate future insertion into real-world systems. Finally, Dr. Melanie Cole, Rodman Materials Research Laboratory (Army Research Lab) is working with us to establish processing methods for integrating diamond and ferroelectric thin-films.

References:

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