

## CURRICULUM VITAE

### PERSONAL DATA:

**Name** **SAMAR MOUSTAFA ABD-ELNAEEM ABD-ELRAHEEM**

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Faculty of Science  
Assiut University  
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### EDUCATION:

University of Kanazawa  
*Department of Electrical  
Eng. and Computer  
Science* Ph.D degree in Electronic Materials and Devices  
(Physics)  
Title of the dissertation: (**Computational studies on  
adsorption behavior of hydrogen- and oxygen-  
related species on diamond (111) surfaces**)  
Supervisor: **Prof. Takao Inokuma**

University of Kanazawa  
*Department of Electrical  
Eng. and Computer  
Science* M.Sc. Physics sciences (Electronic Materials and  
Devices) 2011

Assiut University, Egypt B.sc Degree in Physics 2006

### ACADEMIC APPOINTMENT:

From Jan. 2007  
To Till now Instructor at Physics Department, Faculty of science, Assiut  
University, Assiut, Egypt

From April. 2011  
To March 2014 Graduate student in the Department of Electrical Eng. and Computer  
Science, Kanazawa University, Japan.

From June 2014  
Till now

Teacher at Physics Department, Faculty of science, Assiut University,  
Assiut, Egypt

## **PUBLICATIONS:**

**Samar Moustafa**, Norio Tokuda, and Takao Inokuma, “Density Functional Studies of Surface Potentials for Hydrogen and Oxygen Atoms on Diamond (111) Surfaces”, *Jpn. J. Appl. Phys*, Vol. 53, pp. 02BD01-1-02BD01-4. (2014).

**Samar Moustafa**, Norio Tokuda, and Takao Inokuma, “Density Functional Studies of Surface Potentials for Hydrogen and Oxygen Atoms on Diamond (111) Surfaces”, Proc. Int. EM-NANO Conf., Kanazawa, pp. 201 (2013).

## **RESEARCH**

### **M. Sc. Research**

Si nanocrystals embedded in SiO<sub>2</sub> matrix have attracted a great attention, due to their high stability and possibility of emitting visible light at room temperature. Thus, thin silicon oxide films SiO<sub>x</sub> (0 ≤ x ≤ 2) are present in many microelectronic and optoelectronic applications such as silicon-based light emitting diodes (LEDs) and optical sensors.

During my Master, we investigate that the r.f. sputtering of a Si/SiO<sub>2</sub> target in Ar plasma is a useful method for depositing SiO<sub>x</sub> films with a continuous control of the Si concentration. Also, we propose hydrofluoric acid (HF) solution treatment to improve the luminescent efficiency and electrical properties of SiO<sub>x</sub> films.

SiO<sub>x</sub> films were deposited by a sputtering system with a 13.56 MHz r.f. source. The deposited films were annealed at 1100°C in an N<sub>2</sub> atmosphere for 1 h to induce the formation of Si nanocrystals embedded in the insulating matrix. Then, the film was etched with diluted hydrofluoric acid (DHF) to reduce the oxide layer covering the nc-Si particles (this solution had a selective effect on the structures; specifically, the solution dissolved the oxide matrix and did not etch nc-Si particles). Au electrodes were evaporated on the top and the bottom of the samples. The composition, morphology, electrical, and luminescence properties were investigated by Fourier transform infrared absorption (FTIR), atomic force microscopy (AFM), I-V characteristics and photoluminescence (PL) measurement, respectively.

The PL results after etching showed that the main peak intensity decreases after etching and shifts to the shorter wavelengths in the spectrum and there is one more low-intensity band in the region of shorter wavelengths between 550 nm and 650 nm. The AFM images of the etched sample showed that there are nc-Si particles on the etched surface. The dc current–voltage (I-V) characteristics were measured before and after etching with DHF. It was observed that the etched sample showed higher current density than non-etched one.

The electrical characteristics of SiO<sub>x</sub> were improved by using DHF. This can be achieved through lowering of resistivity resulting by reduction of oxide layer surrounding nc-Si particles.

### **Ph. D. Research**

Diamond is an allotrope of carbon that has become one of the most important materials in industry. Because of its many outstanding physical and chemical properties, such as high thermal conductivity, extreme hardness, high transparency for ultraviolet-infrared (UV-IR) radiation, chemical inertness, and low friction coefficient, it has been a very useful material for various technological applications. Nowadays, the chemical vapor deposition (CVD) is the main method to grow diamond film. In the epitaxial growth of diamond, three low-index faces, (111), (110) and

(100), are the main orientations. Among the three orientations, (111) surface is of particular interest because the formation of atomically flat surfaces has been realized by utilizing a lateral growth mode on the (111) face.

Adsorption of foreign atoms on diamond surface can significantly modify its physical and chemical properties. These adsorbates play an important role in thin-film growth by affecting, for instance, adatom adsorption, nucleation and migration on surfaces. The most common species that terminate diamond surfaces are hydrogen- (H) and oxygen-related species (e.g., O and OH groups). It has been shown that hydrogenated diamond surfaces can preserve its unique p-type surface conductivity and exhibit significant negative electron affinity. On the other hand, oxygenated surfaces show no surface conductivity and shift the electron affinity from negative to positive. These effects of hydrogen and oxygen to modify the surface properties of diamond are very attractive for use in electronic applications such as Schottky diodes, field effect transistors and pH sensors. Also, adsorbed oxygen atoms on diamond surfaces have also been known to make them hydrophilic while hydrogenated surfaces are hydrophobic.

Also, the investigation of hydrogen and oxygen coexistence on the diamond surfaces could also be important. Previous studies have established that the diamond surface terminated with OH exhibits a negative electron affinity, which makes the material potentially useful in a number of applications, such as photocathodes and cold cathode emitters.

The interaction of hydrogen, oxygen and Hydroxyl group on diamond surfaces becomes an important issue for both diamond technology and surface science study. However, their behaviors on diamond surfaces seem not to be understood enough. In this study, the potential energies for neutral H, O atoms and OH group on a flat and stepped (a surface with monoatomic step) diamond (111)-(1×1) surface are investigated by a molecular orbital method based on the density functional theory (DFT) in order to clarify the static aspects for the interaction between those adatom and the surface.

Two-dimensional profiles of the potential energy for hydrogen, oxygen atoms and hydroxyl group are presented. The behaviors of surface diffusion and the influence of atomic steps are discussed. The oxygen adatom is found to have much lower energy barrier for migration. On the basis of the variations of potential energy, surface diffusion coefficients of adatoms are calculated. The potential energy for the O adatom is much lowered near the step edge. It is suggested that the oxygen atoms adsorbed on diamond (111) surface favor to be trapped near an atomic step after migration. Also, relaxation of the stepped surfaces with H adatom, O adatom, OH group as well as bare surface was studied. It was found that the carbon atoms at the step edge, which are bonded to with H adatom or OH group, reconstructed to lower the surface energy and forms a downward slope in the (112) direction.

## **TECHNIQUES:**

Working in this lab made me familiar with the following techniques;

1. Preparation of  $\text{SiO}_x$  thin film by sputtering
2. Measurements of electrical and optical properties of thin films.
3. Familiar with using atomic force microscope (AFM).
4. Electron Microscope.
5. Computer simulation calculations using ORCA software, OCTAVE..etc .

## **MEMBERSHIP:**

The Japan Society of Applied Physics (JSAP).