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Simulation of Au and Mo Nanoparticles Effects

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Abstract: ***I report a theoretical study of the behavior of Au nanoparticles anchored onto a Si (111) substrate and the evolution of the combined structure with annealing and oxidation. By simulation of the data which is noticed in reference [1] and using the Matlab program with curve fitting to conclude Au nanoparticles, formed by annealing a Au film, appear upon a growing layer of SiO2 during oxidation at high temperature. Deposition of molybdenum oxide Mo (3d) on Ag (111), The surface concentration of Mo which is calculated from the XP peak area using methods which described [2,3]respectively, where we discuss these results by using a curve fitting method that is a theoretical method to test the system. Gold, the archetypal noble metal, is usually associated with an inhibition of surface reactivity by site blocking. In addition, we show that the simulation of this study extends to analysis the on Cu (100) surfaces a gold adlayer can actually increase the extent of reaction with the substrate. We note that the theoretical results are agreeted with the experimental results and this work expanded the ranges of temperature and binding energy with intensity in the case of Au/Sio2 and the effects on the binding energy and concentration with increasing time to limit range for Mo/Ag(111) and the structure of Au/Cu(100).***

Keywords: Intensity, Binding Energy, Concentration, Temperature Effect

1. Introduction

Metal nanoparticles on semiconductor or oxide surfaces are of great importance in catalysis, semiconductor fabrication, sensors, and even in anticancer therapies and nanotoxicology [3]. In catalysis, for instance, such nanoparticles are often the active phase in the reactions involved, and gold, the subject of this paper, has become a focus of enormous interest in catalysis in the last 20 years.

In addition to their unique electronic properties, nano-materials have advantageous physical properties that have been utilized in a variety of different applications. Their high surface area, high physical strength and low weight make them ideal support surfaces for uses ranging from nano-oscillators to heterogeneous catalysts. A common factor in all such applications is the need to control the interface between nanometal and substrate that need to bind to it. The nature of that interface will be dependent on the structure and functionality of the carbon surface and many applications of carbon materials apply empirically developed treatments to modify the surfaces concerned. Behavior of nanoparticles is perhaps of even greater importance for the huge technological area of semiconductor devices and their fabrication. The discrete nature of Au nanoparticles also attracts a lot of interest in the manufacturing of portable diagnostic devices based on local surface plasmon resonance (LSPR)[4].As in catalysis, the integrity of such fine structures is crucial to performance, and this integrity becomes more difficult to maintain as the features become even smaller because of the increased relative importance of atomic diffusion and hence loss of prefabricated structure.

There are other operation such as electrodeposition of lanthanum hydroxide films onto nickel substrates in the presence of polyethylenimine (PEI) has been studied by infrared spectroscopy, x-ray photoelectron spectroscopy and atomic force microscopy with the aim of exploring the effectiveness of the technique and the chemistry of the deposited films. Maximum deposition rates were recorded for low concentrations of PEI with rates decreasing at higher PEI concentrations largely because of the poor structural integrity of the deposited films. Similarly, extending the deposition times did not improve film coverage as thicker films adhered less well to the nickel substrate. The deposited films were shown to contain co-deposited PEI with the concentration remaining constant within the films during deposition, but changing linearly with PEI concentration in the depositing solution [5].

Mechanistic aspects of catalytic oxidation at metal surfaces have involved four distinct stages of investigation which, in chronological order, are: (a) oxygen chemisorption and surface reconstruction with evidence for discrete metal and oxygen states; (b) the reactivity of specific oxygen states in oxydehydrogenation reactions; (c) the chemistry under dynamic conditions with evidence for dioxygen–reactant complexes at low temperature; (d) atom resolved evidence from scanning tunnelling microscopy[6-8].As described in the introduction, metal oxides are key components of a wide range of industrial catalysts. Since catalysis occurs mainly on the surface, the surface properties of the metal oxides assume great importance. The study of the field of metal-oxide surface structures is quite young compared to that of metals or semiconductors. The applications of several ultra-high-vacuum (UHV) techniques in the last 20 years have led to a surge of interest in the study of metal oxide surfaces.

There are several reasons for the lag in the growth of knowledge of metal oxide surfaces. The electronic structure of metal oxides is much more complex than that of metals or semiconductors. The number of atoms per unit cell along with the reduced symmetry at the surface and the necessity to separate the surface and bulk effects makes the task of evaluating the surface properties of the metal oxides a daunting one. Another difficulty is a practical one related to experimental techniques used by surface scientists.

2. Theory

In this paper I introduce the theoretical study of nanoparticles such as Au/SiO_2, Au/Cu (100) and Mo/Ag (111). By using the Mat-lab program with curve fitting method, one can find results enhance the experimental

results [1-3] which can be introduced for all cases. Au and Mo nanoparticles metals are assembled in different types of substrates.

A theoretical method to study Au and Mo nanoparticle that self-assembly in different substrates was demonstrated. Au films and nanoparticles on single-crystal alumina [1] and showed that there was little evidence of sintering, the film behavior being dominated by dewetting above 400 °C and by thermal evaporation above 1000 °C. In this work we look at the effect of changing the substrate to single-crystal Si, and we report very different behavior, especially in terms of the effect of thermal treatment which results in partial encapsulation of Aunanoparticles on the single-crystal Si. When using the Matlab program to find the equation that describes the most effects of binding energy and intensity with temperature and for a time.

In this research, we introduce the theoretical method for Matlab program and addition to introducing the experimental results of assembled for example Au/SiO_2. The equations which acts the effects between the variables for each model are expressed in the next section with the ranges of the factors of the three types of structures. Once the molybdenum oxide layer thickness exceeds [3] mono layers this oxidation pathway for the molybdenum oxide is closed off, and reduced Mo states begin to appear at the surface. When explored a range of gold concentrations on Cu(100) surfaces and these will be described in a more lengthy and detailed publication in the near futureAu(4f) spectrum for Au evaporated onto the clean Cu(100) surface.

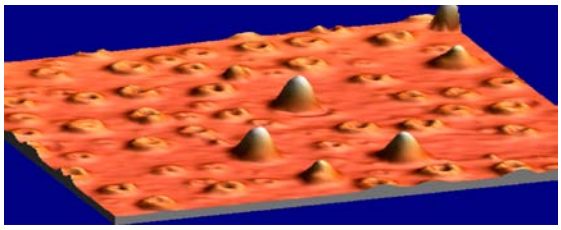

Figure 1: Au nanoparticles anchored on a SiO_2 substrate [1].

Figure 4. Schematic diagram of the oxidation of the Si crystal (shown in red) in the absence (a) and presence (b) of Au nanoparticles. In (a), as oxidation proceeds, the SiO2 layer (shown in green) grows, and this must occur by net transport of Si outward from the original surface.

Because the density of the two phases is similar, but the SiO2 layer is about 50% as dense in Si as the Si crystal itself, the SiO2 layer grows both out of the original surface plane and down from that layer into the bulk. When nanoparticles are present (b), here showing a smaller and a larger nanoparticle, then the tendency is for them to "float" on the growing SiO_2 and also to become encapsulated in different degrees.

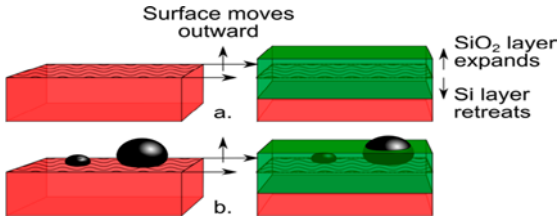

Figure 2: Self-assembled of Au nanoparticles on SiO_2 Substrate, i.e, which assembled under oxidation proceeds of Si [1].

3. Results and Discussion

By using the numerical analysis for the different metals we estimated that there are boundary limits to varying the parameters of each system in this study, which can be shown as the three cases of the systems. In this type of numerical methods, the equation equation which is estimated from the curve fitting method expresses the relation between the variables of the system through the study and by using this equation we can be predicted the results and the variety of the situations for the system.

3.1 Au Nanoparticles on a Silicon Wafer During Thermal Oxidation

When studying the effects of temperature increasing in the intensity and binding energy together, I find that intensity increases with increasing temperature to 1500 ^{o}C an increased energy increases in the limit range. These variables agree with the experimental study [1] but I study these effects at limit ranges. The intensity is arrivingtoo fast increasing at critical temperature (1400 ^{o}C). The range of variation of binding energy and temperature is summarized in Table 1. Figure, 3shows the of binding energy with temperature on Au/Sio_2.Figure,4 shows binding energy and intensity with increasing temperature are shown in, and Figure 4. The polynomial function which describes the effect of temperature on binding energy (BE) and intensity is given by the bolonomial equation which is produced from using the curve fitting to the experimental data

$$I = 2.8BE^{4} - 9.4\times10^{2}BE^{3} + 1.2\times10^{5}BE^{2} - 6.6\times BE + 1.4\times10^{8} \quad (1)$$

Where I am the intensity.

Table 1 summarizes the results of variations of bindingenergy with intensity at the limit ranges

Table 1: Results of variations of binding energy with intensity at the limit ranges

Binding Energy (eV)	*Temperature (C^o)*
80	100
86	1500

3.2Study of the effects which result from deposition of molybdenum oxide Mo (3d) on Ag (111)

We study the effect of concentrations (cps) of Mo with binding energy where we note that the binding energy arrived to critical value which corresponding to high value of cps. Table 2 summarizes the results of variations of binding energy with intensity at the specific values. The equation which describes the effect of the binding energy with concentration (cps) is given by the bolonomial equation which is produced from using the cuve fitting to the experimental data

$$cps = 0.0002\,BE^{4} - 0.058BE^{3} - 1.7\times10\ \ BE^{2} + 2.74\,BE + 0.5027 \quad (2)$$

Figure 6, shows the variation of binding energy with increasing the concentration

Table 2: Results of Variations of Building Energy with Concentraction at the Specific Values.

cps	*Binding Energy eV)*	*Time (min)*
5×10^{10}	226	10
10×10^{10}	240	200

3.3 Au(4f) spectrum for a concentration of Au at the clean Cu (100) surface

There are many results are calculated from the spectrum of Au for different concentrations with different times and at limit values of binding energy ,we note that limit range of values of binding energy with high value of concentration. Table 2 summarizes the results of variations of binding energy with intensity at the specific values. The equation which describes the effect of the binding energy with concentration at different of times is given by

$$cps = 0.005\,BE^{4} + 4.8BE^{3} - 1.7\times10^{3}\,BE^{2} + 2.7\times10^{5}\,BE - 1.6\times10^{7} \quad (3)$$

Figure 7, shows the variation of binding energy with increasing the concentration at different times.

Table 3: Results of Variations of Building Energy with Concentaction at the range of Specific Values.

cps	*Binding Energy (eV)*
17	72
24	80

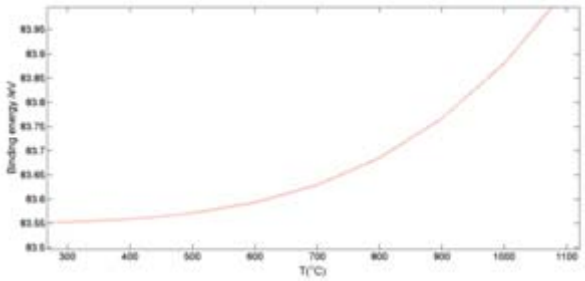

Figure 2: Variation of binding energy with temperature on Au/SiO_2

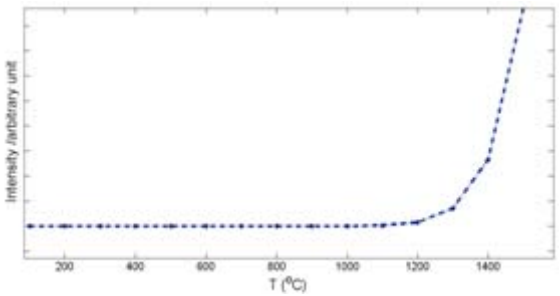

Figure 3: Variation of intensity with temperature on Au/SiO_2

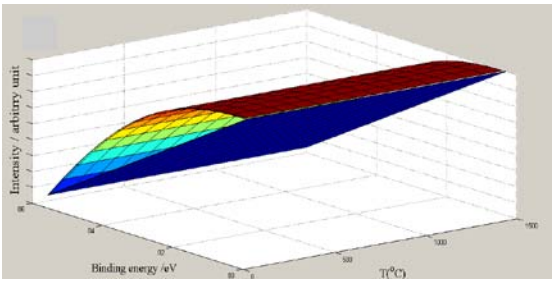

Figure 4: Three dimensionalplot for effects onAu/SiO_2

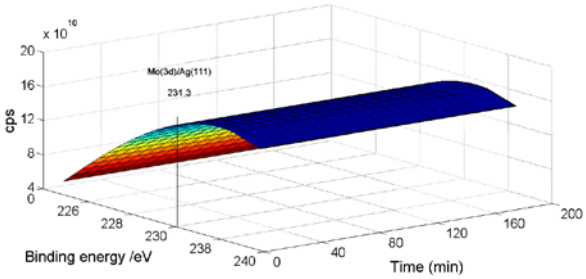

Figure 5: Three plot for effects on Mo(3d)/Ag(111).

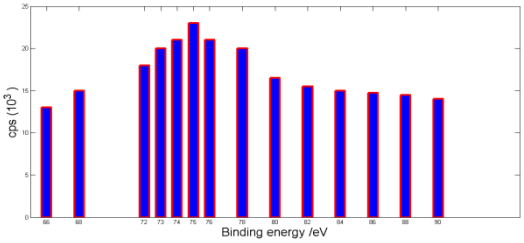

Figure 6: Three plot for effects on Au/Cu(100).

All these results refer to the same behavior of the intensity curves for different tree structures and for different ranges of parameters of each system.

From the above results we note that there is characteristic values for intensity and limit values of binding energy at range of temperature of Au/SiO2 and also for the other two types of structures where the intensity and binding energy in these structures are changed through the time.

4. Conclusions

Actual applications require careful weighing of all the parameters. We conclude that the overall performance of the concepts is better than that of the other concepts. In this work the results are summarized the effects of three types of nano particles, which assembled on different types of substrates. The effective nature of Au and MO on the underlying groups of materials that allow for chemical nano patterning, through the selective modification of the amine groups not involved in the binding interaction with the nano particles, to generate nano particles on the different substrate surfaces.

We note that the same behavior of intensity variation in these systems types. We note that the Au and Mo nanoparticles, which assembled in different metals produced variations and effects between three variables such as intensity, binding energy and temperature for Au/SiO2[1] and the same variables but these variables are changed with time such as Mo/Ag(111)[2] and Au/Cu(100)[3]. We observe that the results are agreed the work of researches [1-3] and we expand this work theoretically to different ranges of

variables such as temperature and concentration of the nanoparticle metal which assembled on the surface of substrate. We note that the there are maximum value of the intensity of limit value of the binding energy with high temperature in the case of Au/SiO_2but this value of intensity is greater when the temperature increasing with the limit value of building energy. In the case of study the maximum value of concentration with the range values of binding energy for 200 min in the case of Mao/Ag (111) and for Au/Cu (100) we estimate that the relation between concentration and binding energy where we note that there is a maximum value on concentaction with limit value of the binding energy at the range in in this study.

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