

The effects of Palladium, Gold, and Iron Nanoparticles as Medical Catalysis

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Abstract: Thin layers and nanoparticles of metals on or oxide surfaces are of great importance in catalysis, sensors, and even in anticancer therapies and nanotoxicology. The applications of the metals that are studied in this study act the one of the important techniques in the biological science and medicine. Cancer nanotherapeutics are rapidly progressing and are being implemented to solve several limitations of conventional drug delivery systems such as nonspecific bio distribution. To improve the bio distribution of cancer drugs, nanoparticles have been designed for optimal size and surface characteristics to increase their circulation time in the bloodstream. We report a theoretical study of the behavior of Au, Pd and Fe nanoparticles anchored onto γ -Fe₂O₃ substrate. By simulation of the data which is noticed in reference of Philip R. Davies et.al and using the Matlab program with a curve fitting method to study the effect of increasing the Au nanoparticles appear upon a growing layer of γ -Fe₂O₃ through limit time. We discuss these results by using a curve fitting method that is a theoretical method to test the system. It is noticed that the theoretical results are in agreement with the experimental results and this work expanded the ranges of kinetic energy with intensity in the case of Au, Pd and Fe on γ -Fe₂O₃.

Keywords: Intensity, Binding Energy, Concentration, Temperature Effect.

I. Introduction

The recent study of the effects of performance and structure highlights the importance of the oxidation state of Pd on the catalyst surface. Nanogold supported on TiO₂ or is the most active material for low-temperature oxidation, and it has recently been used for other important applications such as peroxide synthesis and selective oxidation reactions [1,2]. Furthermore, a major problem in catalysis is the stability of nanoparticles, which is limited at elevated temperatures because of a variety of ripening processes [3,4]. Using a combination of STM and LEIS spectroscopy the fabrication of Au/Pd bimetallic nanoparticles supported on γ -Fe₂O₃ using metal vapor deposition under ultra high vacuum. Au and Pd particles were sequentially deposited onto the iron oxide substrate and after brief thermal treatment the two species alloyed to form Au-Pd core-shell particles [2]. These supported particles could be used as models for real Au-Pd catalysts to explore mechanisms which are highly active for numerous reactions [2,5]. A simple and efficient principle for nanopatterning with wide applicability in the sub-nanometers regime is chemisorption of nanoparticles; at homogeneous substrates, particles carrying surface charge may spontaneously self-organize due to the electrostatic repulsion between adjacent particles. Gold surfaces modified with monolayers of functional thiols or disulfides [1] are often used for analytical purposes, not at least for biosensor applications [3] or as models for investigation of biological surface interactions [6]. Methods used to identify functional groups include temperature programmed desorption (TPD) and infrared spectroscopy (IR) but the former is a rather indirect probe and IR is only reliable for the identification of functional groups with strong transition dipoles [7]. It is possible for minority species to dominate the infrared spectrum whilst the majority state is undetected [1,3]. Although they were able to demonstrate the importance of the oxygen functionality at the surface the authors were unable to distinguish between the roles of the different possible oxygen groups in the attachment of the gold. Nanoparticles could be sintered into the substrate by gentle heat treatment prior to modification with these, giving a chemically homogeneous, but nanostructured interface [8,9]. Using this approach, the adsorption of charge-stabilized gold nanoparticles onto the modified surfaces is randomized, but the distance between adjacent particles will reflect their mutual electrostatic repulsion [9]. At saturation, the particle coverage can therefore be tuned by controlling the ionic strength of particle solution, thereby altering the Debye screening of the particles' surface charges [10-15]. The researchers report how such electrostatic control can be used for the deposition of nanoparticles in gradient nanopatterns, induced by controlling the diffusion of ions into a particle solution [5].

II. Theory

Metal oxides, in particular transition metal oxides, exhibit a wide-ranging array of properties and phenomena [1,16]. The diverse structures adopted by the metal oxides are helpful to demonstrate the relationship between structures and properties [1,2]. Correlation of structure and physical properties of transition

metal oxides requires an understanding of the valence electrons that bind the atoms in the solid state. The band theory and the ligand field theory have been invoked to explain the electronic properties of transition metal oxides [1,12]. The important properties of oxides that are of interest are magnetic, electrical, dielectric, optical, Lewis acid/base, and redox. Oxides in heterogeneous metal catalysts facilitate well-observed phenomena such as hydrogen [6,7]. Surface science of metal oxides has received tremendous attention during recent years. The advent of several advanced techniques to probe their surfaces has led to a new understanding of their surface properties and structures [17-20]. This in turn has helped catalyst scientists to tailor the properties of the oxidized materials for appropriate applications [5-9]. In this paper I introduce the theoretical study of nanoparticles such as Au/ γ -Fe₂O₃, Fe/ γ -Fe₂O₃ and Pd/ γ -Fe₂O₃. By using the Mat-lab program with curve fitting method, one can find results that enhance the experimental results [1,2] which can be introduced for all cases. Au, Pd and Fe nanoparticle metals are assembled in the same substrate. A theoretical method to study Au, Fe and Pd nanoparticle that self-assembly in the same substrate was demonstrated [2]. 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/ γ -Fe₂O₃, Fe/ γ -Fe₂O₃ and Pd/ γ -Fe₂O₃ where.

The effects lead to differentiating between nanoparticles of different composition related to the experimental strategy of Au and Pd particles with different and distinct sizes. Our theoretical results agree with experimental data.

III. Results and Discussion

Au Nanoparticles on γ -Fe₂O₃ : When studying the effects of increasing in the intensity and kinetic energy together with time, we find that intensity increases with increasing the kinetic energy that increases in the limit range. These variables agree with the experimental study [2] but I study these effects at limit ranges. The intensity is arriving too fast increasing at critical domain. The polynomial function which describes the effect of temperature on kinetic energy (KE) and intensity is given by the polynomial equation which is produced from using the curve fitting to the experimental data

$$I = 8 \times 10^{-6} KE^4 - 0.029 KE^3 + 40 KE^2 - 2.4 \times 10^4 KE + 5.5 \times 10^6 \quad (1)$$

Where I is the intensity.

Study of the effects which result from deposition of Fe on γ -Fe₂O₃: We study the effect of concentrations (cps) of Mo with a binding energy where we note that the binding energy arrived to critical value which corresponding to the high value of intensity. The equation which describes the effect of the binding energy with intensity (cts/s) unit is given by the polynomial equation which is produced from using the curve fitting to the experimental data

$$I = -3.5 \times 10^{-6} KE^4 + 0.012 KE^3 - 15 KE^2 + 8.2 \times 10^3 KE + 1.7 \times 10^6 \quad (2)$$

Spectrum analysis of Pd/ γ -Fe₂O: There are many results calculated from the spectrum of Au/ γ -Fe₂O₃ for intensity with different times and at limited values of binding energy, we note that limit range of values of kinetic energy with high value of intensity. The equation which describes the effect of the kinetic energy with intensity at different of times is given by:

$$I = 8.8 \times 10^{-7} KE^4 - 0.0031 KE^3 + 4 KE^2 - 2.3 \times 10^3 KE + 4.9 \times 10^5 \quad (3)$$

The range of variation of kinetic energy and intensity with time is summarized in Table 1. Figure, 1 shows the variation of intensity with time on Au/ γ -Fe₂O₃. Figure, 2 shows to the variation of kinetic energy and intensity Au/ γ -Fe₂O₃. Figure 3 represents the effect of the increasing of kinetic energy with intensity with time (1-2 minute) on Au/ γ -Fe₂O₃.

Table 1, summarizes the results of variations of kinetic energy and intensity with time at the limit ranges. Table 2, summarizes the results of variations of binding energy with intensity at the specific values.

Table 1: Results of variations of kinetic energy in intensity at the limit ranges

Intensity (cts/s)	Kinetic Energy (eV)	Time (min)
1000	875	1
2200	1000	2

Table 2:Results of Variations of kinetic Energy with intensity at the Specific Values.

Intensity (cts/s)	kinetic Energy (eV)	Time (min)
2800	725	1
4800	900	2

Table 2 summarizes the results of variations of kinetic energy with intensity at the specific values. The equation which describes the effect of the kinetic energy with intensity at different of times is given by:

$$I = 8.8 \times 10^{-7} KE^4 - 0.0031 KE^3 + 4 KE^2 - 2.3 \times 10^3 KE + 4.9 \times 10^5 \quad (3)$$

Table 3: Results of Variations of Kinetic Energy with intensity (cts/s) at the range of Specific Values.

Intensity (cts/s)	kinetic Energy (eV)	Time (min)
1600	825	1
2200	900	2

Figure 4, shows the variation of kinetic energy with increasing the intensity, and Figure 5 shows the variation of kinetic energy with increasing the intensity (cts/s) at different times.

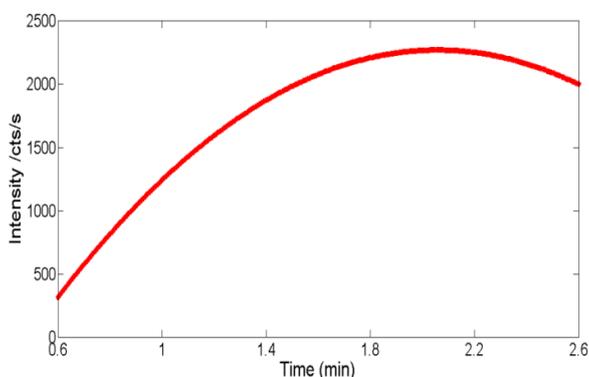


Figure 1: Time variation of intensity of Au γ -Fe₂O₃ structure.

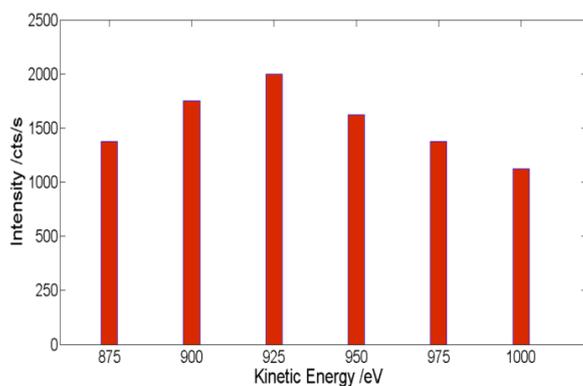


Figure 2: Variation of intensity with kinetic energy of Au/ γ -Fe₂O₃ structure .

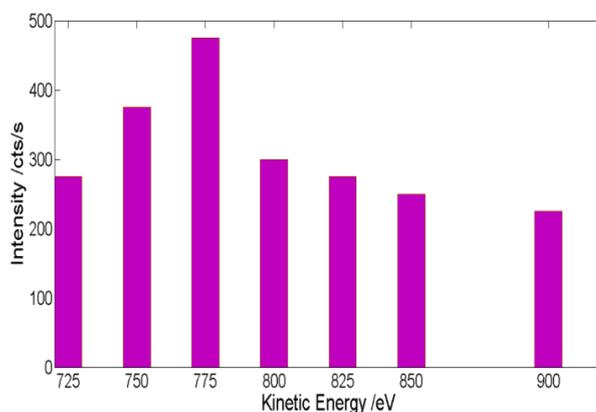


Figure 3: Three dimensional plot of the variables variation on the Au/ γ -Fe₂O₃ structure .

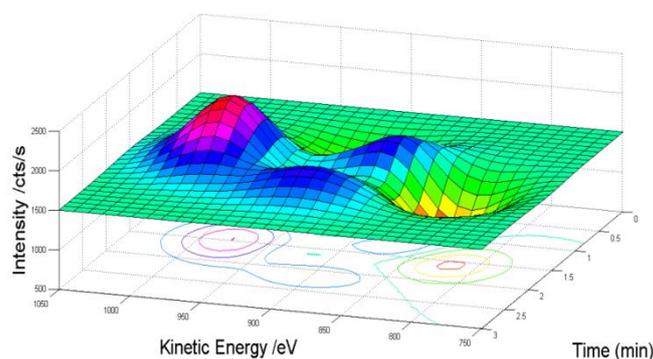


Figure 4: Variation of intensity with kinetic energy of Fe/ γ -Fe₂O₃ structure.

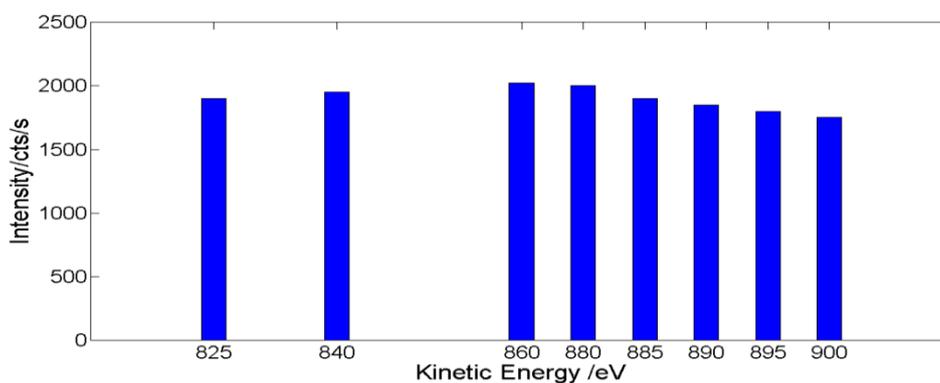


Figure 5: Variation of intensity with kinetic energy of Pd/ γ -Fe₂O₃ structure.

IV. Conclusion

More applications require careful weighing of all the parameters. We conclude that the overall concepts are better than that of the others. In this work the results summarize the effects of three types of nanoparticles, which assembled on the same substrate (-Fe₂O₃). We notice that our theoretical results agree with the experimental results and for the different range the same behaviors are noticed. When using the Matlab program with curve fitting method, we note that Fe metal is larger affected by increasing the kinetic energy with time when it compared to Pd and Au. The reason for this behavior of Fe is produced from the matching between the Fe and the substrate. The simulation of these structures is lead to be predicted by the spectrum of these structures at different ranges of variables. We observe that there are critical values of intensity which are corresponding to the limit values of kinetic energy for each of our structures. But, the maximum intensity values of all structures are different. One each of three types of structures (Au/ γ -Fe₂O₃) is important in the medical catalysis where Au is used in the treatment of cancer.

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