

Theoretical Treatment for the Ion Sputtering Process from Quantum Dot Surface

J. M. Al-Mukh and A. R. Ahmed

Department of Physics – College of Education for Pure Sciences – University of Basrah

Abstract

In this study, simple theoretical treatment is presented to calculate the neutralization and excitation probabilities throughout the ground state channel and the throughout the excited state channel for atom sputtered from quantum dot surface. The system energy levels considered in our treatment are just the levels lying within the energy window. The Hamiltonian that describes the system is written taking into account the ground and the excited states of the sputtered atom as well as the electron scattering process (i.e. the electronic excitation) within the quantum dot energy band levels. We get use of Heisenberg equations of motion to derive the equations of motion that describe the system. The law of charge conservation is investigated. The set of related equations are solved numerically. The effect of electronic excitation within the quantum dot band energy is highlighted and discussed.

1- Introduction

There has been great effort to interpret the microscopic dynamics of surface roughness and pattern formation induced by ion sputtering (S. Facsko *et al.* 1999). The characteristic period in the submicrometer to nanometer range is defined by the sputtering conditions (Abathr R. Ah. Al-Ebade. 2009) (for example ion energy, ion flux, and substrate temperature) and by the material properties. The controlled fabrication of semiconductor nanostructures remains a key requirement for the development of future optoelectronic and electronic devices (S. Facsko *et al.* 2001). Quantum dot structures are supposed to form the building block of future electronic devices like quantum cellular automata or single electron transistors. The main bottleneck in the application of quantum dots is the difficulty of creating ordered structures with a high uniformity in size and of crystallinity (T. Bobek *et al.* 2001). The production of semiconductor nanostructures has attracted the interest of many research groups because of the important applications in optoelectronic and quantum devices.

Many of the interesting materials properties depend on the size, shape and regularity of the nanometric substructure. In particular, efficient light emission from

silicon is achieved when the nanostructures are smaller than the bulk exciton (E. Chomski and G. A. Ozin. 2000, L. Pavesi *et al.* 2000, Raul Gago *et al.* 2001).

Techniques such as Si ion implantation, e-beam writing, scanning probe lithography, pulsed laser deposition, laser annealing, low pressure chemical vapor deposition and thermal evaporation have been used to fabricate silicon nanostructures.

However, it is not evident that any of these techniques can be used to simultaneously control purity, uniformity and crystallinity of the nanostructures and to produce these efficiently in a large scale. Thus, new processes of fabrication of silicon nanocrystals are being investigated.

One very promising candidate is irradiation of a monocrystalline semiconductor surface by low energy ions. Modifications of surface morphology induced by energetic ion sputtering are complex phenomena and need attention for better understanding of the evolution processes in the atomic scale (D. Datta *et al.* 2002). Recently a novel sputter erosion technique has added further possibilities of fine-tuning processing conditions in many ways (H. Hofsass, K. Zhang. 2008). This was studied theoretically by using Monte Carlo model and resent over mentioned.

2- The Theoretical Treatment

To calculate the neutralization probability for the sputtered ion through the ground state channel or through the excited state channel throughout the sputtering process from quantum dot surface, we consider the energy diagram that shown in fig. (1). E_a (E_x) represents the atomic energy level of the ground state (excited state). While only two states for the quantum dot surface electronic structure will be taken into consideration. These are the LUMO

(lower unoccupied molecular orbital) and the HOMO (higher occupied molecular orbital). The lower one will be denoted by E_L and the higher one is denoted by E_H , while the other states are neglected. In our work, we study the most important parameters that determine the electronic excitation of the sputtered ion throughout sputtering process, that is the electronic excitation in the quantum dot surface energy band levels.

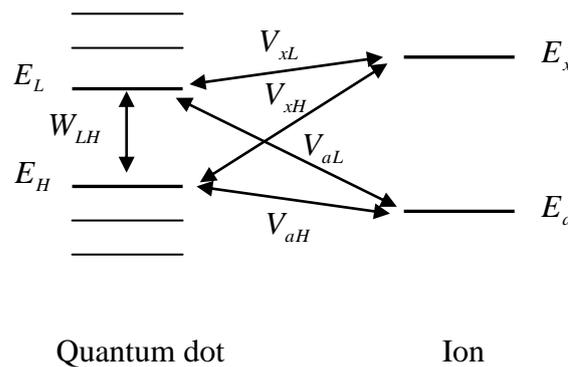


Fig. (1): Energy diagram for ion sputtered from the quantum dot surface

Incorporating the electronic excitations in the quantum dot surface band W_{LH} , the Hamiltonian operator in the

second quantization formalism is written as (M. Kato *et al.* 1996),

$$\begin{aligned}
 H(t) = & E_L C_L^+ C_L + E_H C_H^+ C_H + E_a C_a^+ C_a + E_x C_x^+ C_x \\
 & + V_{aL} C_a^+ C_L + V_{aL}^* C_L^+ C_a + V_{aH} C_a^+ C_H + V_{aH}^* C_H^+ C_a \\
 & + V_{xL} C_x^+ C_L + V_{xL}^* C_L^+ C_x + V_{xH} C_x^+ C_H + V_{xH}^* C_H^+ C_x \\
 & + W_{HL} C_H^+ C_L + W_{HL}^* C_L^+ C_H
 \end{aligned}
 \tag{1}$$

C_i and C_i^+ represent the annihilation and creation operators for the state i ($i=a, x, L, H$). The first four terms in eq. (1) are concened to quantum dot surface band and the sputtered atom in it's ground and excited states before the coupling interaction is switched on .

$$V_{ij}(t) = \langle i|V(t)|j\rangle \quad i=a, x, j=L, H \quad \dots\dots(2)$$

$V(t)$ is the perturbation term due to interaction between the ion and the quantum dot surface. W_{LH} is the interaction that may attributed to the electron scattering in quantum dot surface energy band

$$\begin{aligned} \frac{dC_a(t)}{dt} &= i[H(t), C_a(t)] \\ \frac{dC_x(t)}{dt} &= i[H(t), C_x(t)] \quad \dots\dots(3) \\ \frac{dC_L(t)}{dt} &= i[H(t), C_L(t)] \\ \frac{dC_H(t)}{dt} &= i[H(t), C_H(t)] \end{aligned}$$

$V_{ij}(t)$ is the coupling interaction matrix elements between the quantum dot surface band states and the atomic energy state of the sputtered ion in its ground state or excited state (D. M. Newns *et al.* 1983) .

To derive the equations of motion , the operators $C_a(t)$, $C_x(t)$, $C_L(t)$ and $C_H(t)$ will be defined by Heisenberg representation which satisfy the following Heisenberg equations of motion (in atomic units) (A. S. Davydov. 1973) :-

Then by substituting the Hamiltomian operator in the above equations and getting use of the commutation relations of operators (Amnon Yariv. 1982) ,

$$\begin{aligned} [C_i, C_j] &= [C_i^+, C_j^+] = 0 \\ [C_i, C_j^+] &= \delta_{ij} \quad \dots\dots(4) \end{aligned}$$

where δ_{ij} is kroniker delta function , we get ,

$$i \frac{dC_a(t)}{dt} = E_a(t)C_a(t) + V_{aL}(t)C_L(t) + V_{aH}(t)C_H(t) \quad \dots\dots(5)$$

$$i \frac{dC_x(t)}{dt} = E_x(t)C_x(t) + V_{xL}(t)C_L(t) + V_{xH}(t)C_H(t) \quad \dots\dots(6)$$

$$i \frac{dC_L(t)}{dt} = E_L(t)C_L(t) + V_{aL}^*(t)C_a(t) + V_{xL}^*(t)C_x(t) + W_{LH}(t)C_H(t) \quad \dots\dots(7)$$

$$i \frac{dC_H(t)}{dt} = E_H(t)C_H(t) + V_{aH}^*(t)C_a(t) + V_{xH}^*(t)C_x(t) + W_{LH}^*(t)C_L(t) \quad \dots\dots(8)$$

These related equations satisfy the following condition (W. L. Clinton and Sepra Pal. 1990) ,

$$\frac{dn_a(t)}{dt} + \frac{dn_x(t)}{dt} + \frac{dn_L(t)}{dt} + \frac{dn_H(t)}{dt} = 0 \quad \dots\dots(9)$$

Which means that the sum of the atomic electron density variation rate for the sputtered ion in the ground state and the excited state due to sputtering process is

$$n_i(t) = C_i^+(t)C_i(t) \quad \dots\dots(10)$$

The system of related equations (5-8) are linear and nonhomogenous , these equations can be solved numerically by using Rung Kutta with physical initial conditions to calculate the neutralization

$$P_{gr}(t) = |C_a(t)|^2 \quad \dots\dots(11)$$

$$P^*(t) = |C_x(t)|^2 \quad \dots\dots(12)$$

3- Results and discussion

In order to solve the set of related equations (5-8), we need to determine the initial conditions which are illustrated in table (1). The black dot in the figure referees to the presence of electron. The

$$\begin{aligned} V_{aj}(t) &= V_{0aj} e^{-\lambda_a t} \\ V_{xj}(t) &= V_{0xj} e^{-\lambda_x t} \end{aligned} \quad \text{with } j=L, H \quad \dots\dots(13)$$

The interactions $V_{aj}(t)$ and $V_{xj}(t)$ are energy independent and $V_{ij}(t) = V_{ij}^*(t)$,

equivalent to the variation rate on the quantum dot surface .

$n_i(t)$ refers to the occupation number of the state $i(=a, x, L, H)$, and is given by

probability $P_{gr}(t)$ and the excitation probability $P^*(t)$ through out the ground state channel and the excited state channel as a function of time by using the following relations respectively :-

energy reference is lying on $E=0$. All the energy levels positions $E_i (i = a, x, L, H)$ are time independent.

The coupling interactions between the considered states are given by:-

where $i=a, x$. The parameters λ_a and λ_x are concern related to the classical trajectory of the sputtered ion in its ground

and excited states respectively , so they are related to the velocity of the sputtered ion. As the neutralization (or the excitation) probability is measured as a function of the sputtered ion kinetic energy regardless of its charge state, i.e. one can consider $\lambda_a = \lambda_x$. But in our work $\lambda_a = 0.0001 \text{ eV}$ and $\lambda_x = 0.0002 \text{ eV}$.

The electronic excitation within the quantum dot surface energy band may be caused by the effect of external time-dependent electromagnetic field or time-dependent phonon bath coupled to the quantum dot. It is self-evident that the interaction W_{HL} depends on energy and time. For simplicity this interaction is considered in our calculation as a constant. The set of related equations (5-8) are solved numerically by using Rung Kutta method, the stability of solutions is checked in each step. The energy levels positions are:

$$E_a = -0.002 \text{ eV}, E_x = 0.001 \text{ eV},$$

$$E_H = -0.001 \text{ eV} \text{ and } E_L = 0.00075 \text{ eV}$$

The coupling interactions between the levels are fixed on:

$$V_{oaL} = 0.002 \text{ eV}, V_{oaH} = 0.004 \text{ eV}$$

$$, V_{oxL} = 0.005 \text{ eV} \text{ and } V_{oxH} = 0.002 \text{ eV}$$

While the interaction which may be attributed to the electron scattering in the quantum dot surface energy band is fixed at $W_{LH} = 0.002 \text{ eV}$. The neutralization probability and the excitation probability

are calculated as a function of time for the cases 1,2,3 and 4. These results are presented in Figs. (1-4). According to our results, important notes are reported. As the ion sputtered from the quantum dot, the probability of neutralization and excitation decreasing or increasing depend on the structure parameters as well as on the system levels occupation at $t = 0$.

The neutralization and excitation probabilities $P_a(\infty)$ and $P_x(\infty)$ are calculated as a function of W_{LH} . These results are presented in Figs. (5-8). In all situations, as W_{LH} increases the ion is sputtered from the quantum dot surface to keep the same initial occupation as if there is no coupling interaction between the quantum dot surface energy band and the levels of the ion. It is obvious that three steps can be considered as a future works. These are:

1. Considering time or / and energy dependence for the interaction W_{LH} .
2. Incorporating the quantum dot surface density of states in calculations.
3. Incorporating the electron-electron interaction on the quantum dot or on the sputtered ion.

Table.(1) Schematic energy diagrams to clarify the cases of the intial conditions at $t_0 = 0$

case	Energy diagram	Intial conditions
1		$C_H(t_0) = (0,1)$ $C_L(t_0) = (0,0)$ $C_a(t_0) = (0,1)$ $C_X(t_0) = (0,0)$
2		$C_H(t_0) = (0,1)$ $C_L(t_0) = (0,0)$ $C_a(t_0) = (0,0)$ $C_X(t_0) = (0,1)$
3		$C_H(t_0) = (0,0)$ $C_L(t_0) = (0,1)$ $C_a(t_0) = (0,1)$ $C_X(t_0) = (0,0)$
4		$C_H(t_0) = (0,0)$ $C_L(t_0) = (0,1)$ $C_a(t_0) = (0,0)$ $C_X(t_0) = (0,1)$

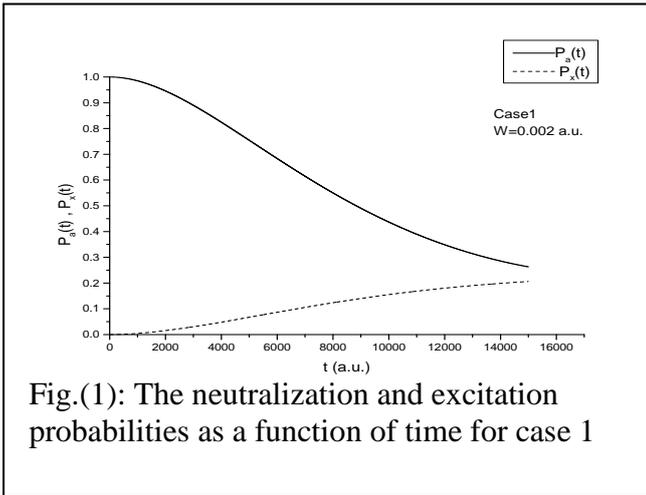


Fig.(1): The neutralization and excitation probabilities as a function of time for case 1

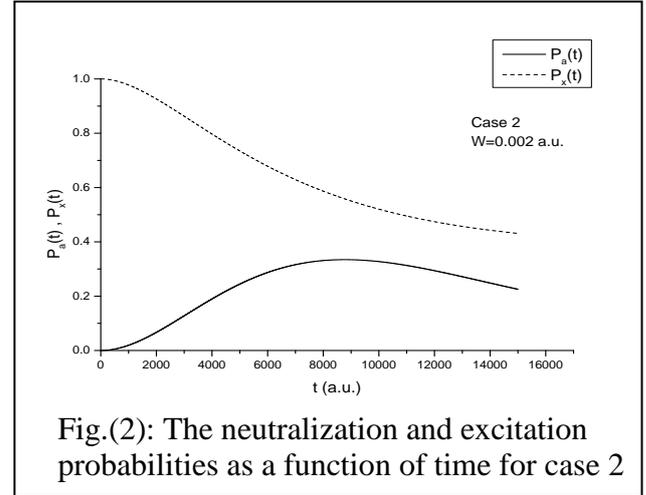


Fig.(2): The neutralization and excitation probabilities as a function of time for case 2

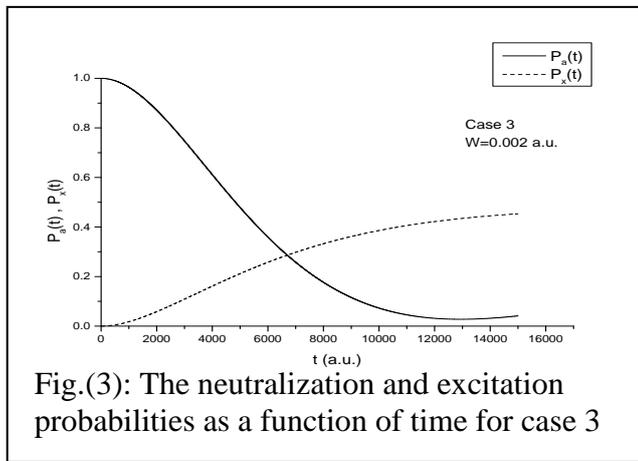


Fig.(3): The neutralization and excitation probabilities as a function of time for case 3

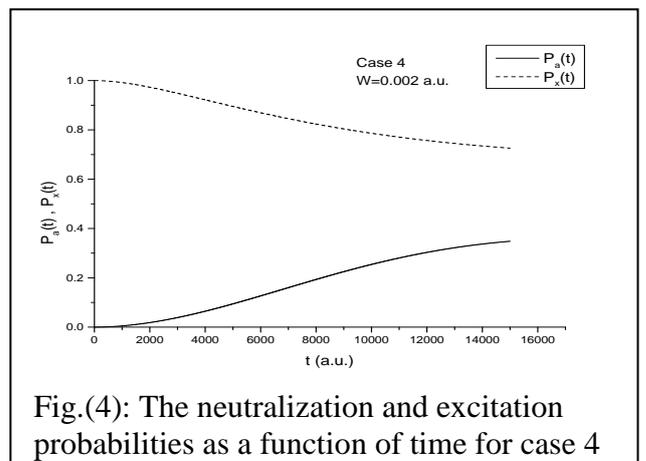


Fig.(4): The neutralization and excitation probabilities as a function of time for case 4

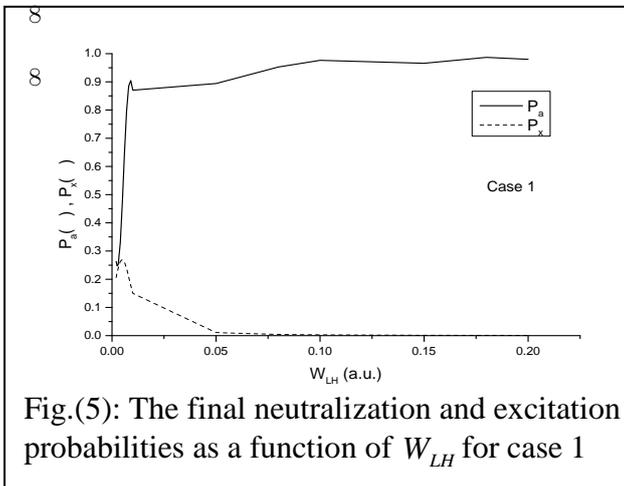


Fig.(5): The final neutralization and excitation probabilities as a function of W_{LH} for case 1

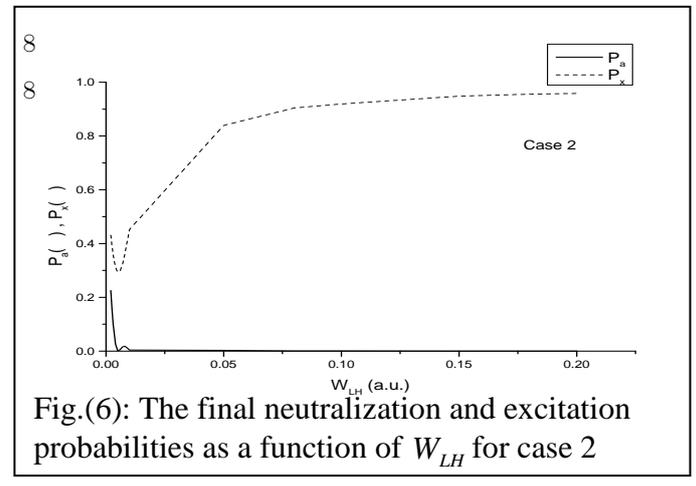


Fig.(6): The final neutralization and excitation probabilities as a function of W_{LH} for case 2

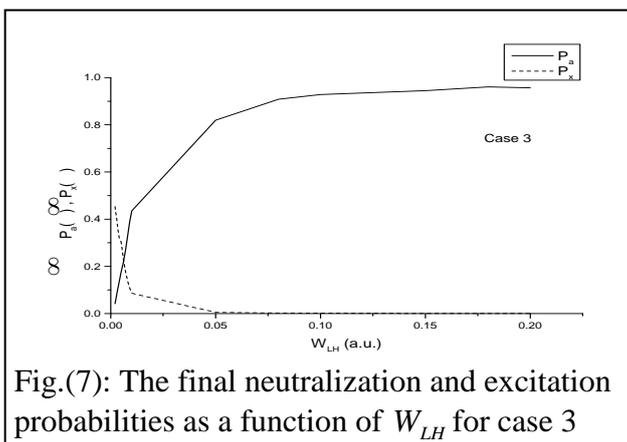


Fig.(7): The final neutralization and excitation probabilities as a function of W_{LH} for case 3

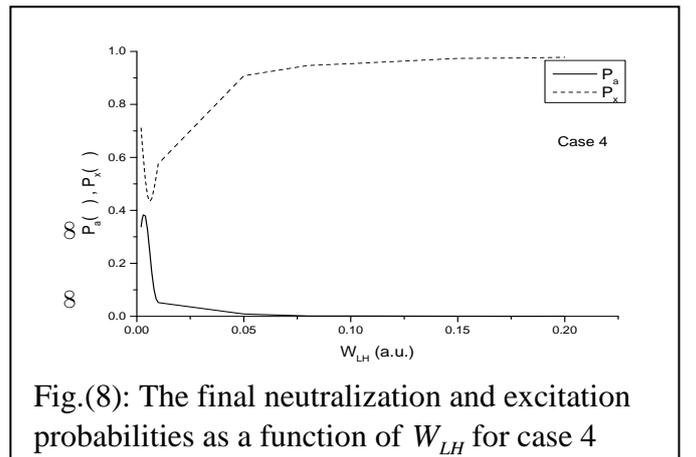


Fig.(8): The final neutralization and excitation probabilities as a function of W_{LH} for case 4

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معالجة نظرية لأيون مقلوع بالسبترة من سطح نقطة كمية

جنان مجيد المخ و أبادر رحمن أحمد

قسم الفيزياء ، كلية التربية للعلوم الصرفة ، جامعة البصرة ، البصرة ، العراق

الخلاصة:

في هذه الدراسة تم تقديم معالجة نظرية لحساب احتمالية التعادل والتهيج خلال قناتي الحالة الأرضية والمثارة لذرة مقلوعة (خلال عملية السبترة) من سطح نقطة كمية. في معالجتنا تم الأخذ بنظر الاعتبار مستويات النظام التي تقع ضمن نافذة الطاقة. كتب الهاملتونين الذي يصف النظام بحيث أخذ بنظر الاعتبار المستويين الأرضي والمثار للذرة المقلوعة بالإضافة إلى عملية استطارة الإلكترون (بمعنى الإثارة الالكترونية) في مستويات حزمة الطاقة لسطح النقطة الكمية. تم الاستفادة من معادلات هايزنبرك للحركة لإشتقاق معادلة الحركة التي تصف النظام، حيث تم فحص قانون حفظ الشحنة. كما تم حل معادلات الحركة عددياً. كذلك ناقشنا وسلطنا الضوء على تأثير الإثارة الالكترونية خلال حزمة الطاقة لسطح النقطة الكمية.