MOLECULAR-DYNAMICS STUDY OF SELF-DIFFUSION: OF THE Au₄;Au₄/Ag(110) SYSTEM

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Abstract: In this work, we will shed light on the results obtained from the molecular dynamics method in the temperature ranging of 300-700K. This investigation concerning the coalescence for the two tetramers islands of system having different forms (SS, TT and NN) deposited at different spacing sites in-channel and cross-channel. The stability of the systems, the diffusion phenomena produced during the dynamics, as well as the diffusion/coalescence lifetime during the evolution of temperature are dependent. The dynamic study shows that between 450K and 650K the homogeneous partial coalescence occurs through the mechanism of the jump. As time goes by increasing the temperature which favors the process of exchange the heterogeneous total coalescence is obtained.

Key words: geometry tetramer 4S, 4N and 4T; island diffusion; evolution dynamic; molecular dynamics simulation.

1. Introduction

The epitaxial growth of a bimetallic surface is rich in dynamic and kinetic phenomenon that attracts the attention of the scientific community that address the problems related to surfaces and interfaces during the growth of thin layers [1-5]. This technology is motivated by a wide range of applications, such as catalytic chemistry, mass transport, microelectronic fabrication, magnetic, photonic and photovoltaic devices [6-12]. During the dynamic evolution of the studied systems, different processes and phenomena are produced. Several experimental and theoretical studies have addressed the mechanisms of diffusion of the elementary elements (adatom, dimer ... islets) responsible for the growth of the surfaces which are the key way to understand this phenomenon on the atomic scale [13-14]. Islands stabilities and adatom dynamics are the main building blocks of thin film growth mode [19-21]. All these phenomena occur via several mechanisms leading to three growth modes: layer-by-layer mode, 3D mode and Stranski-Krastanov mode. These processes include the atoms deposited on substrates, the diffusion of adatoms on surface and the processes of jumps. The latter has been demonstrated experimentally in different systems, such as Ir/W(110), Na/Cu(100), Pd/W(211) [22-24]. Diffusion by exchange process has been observed in different systems as an example Ni/Ni(110) [25]. Nucleation, formation of stable islands and diffusion of dimers and trimers are carried out by these processes. The study by Yi Fu et al. pointed out that the most stable cluster structure is the linear form, but that the energy differences between the linear structure and the other structures for Rh tetramers are smaller than those of Ir tetramers [26]. Surface growth begins with the nucleation of adatoms and dimer, which causes the phenomenon of coalescence by the mechanisms of attachment / detachment of atoms on islands to form a large islands [27-32]. The shape and size of the island play a role in the nucleation and growth of homo systems as well as heteroepitaxial systems. The understanding of the diffusion mechanisms and energetic factors induced by the thermodynamic behavior of the cluster and
the atoms on the surfaces reveals an important interest for the study of the crystal growth and the formation of the films [8] [33-36]. Yi Fu et al. have indicated that the linear chains reach their stability until the number of atoms reach eight atoms [26].

The dynamic diffusion of a single adatom or group of adatoms (clusters) on metal surfaces is a fertile ground for understanding the mechanism of crystal growth and heterogeneous catalysis at the atomic scale [32] [37-39]. While the details of atomic movements are difficult to observe experimentally because the diffusion process takes place over a short period of time; it is, therefore, difficult to follow the diffusion movements of adatoms on a substrate. Molecular dynamics is a useful method for tracking the trajectory as well as the processes that will take place during the dynamic evolution of epitaxy system ad-species [40]. In stage is devoted to the growth of islands by the phenomenon of coalescence [41] [42]. During this growth phase, the two affected clusters are normally larger. The growth of small islands of Au on silver has been studied theoretically and experimentally [43] [44].

In this work, we studied the phenomenon of coalescence for two tetramer islands \( \text{Au}_4 \) on \( \text{Ag}(110) \) by method molecular dynamics. The main axes of this study focused on the stability of the systems, the diffusion phenomena produced during the dynamics, as well as the diffusion / coalescence lifetime during the evolution of the temperature.

In this paper, we described our systems as well as our simulation method in section 2. Then, we discussed the results obtained during the system investigation \( \text{Au}_4 \)/Ag(110) in section 3. Finally, we devoted our attention to a summary in the form of a conclusion.

2. Simulation method

There are many problems in solid state physics requiring the knowledge of the total energy \( E_{tot} \) of a multi-site network according to the profiles \( (\rho_i, r) \) of occupation of these sites by atoms of the same type or binary. In literatures, numerous empirical and semi-empirical models make it possible to model the total energy of the metallic systems as a function of the constituent atoms. In this work, our systems are modeled by a semi-empirical potential based on the Embedded Atom method (EAM) that has been proposed by Foiles et al. [45- 47] . In the approach in question (EAM), the total energy of the system is given by the sum of two terms, one represents the peer interaction that ensures the body-body repulsion of the atomic nuclei in a given cutoff distance , and the other describes the potential of immersing an atom in an electron density. This total energy is expressed by the following formula :

\[
E_{tot} = \sum_i F_i(\rho_i) + \frac{1}{2} \sum_{i<j} \phi_{ij}(r_{ij})
\]

with

\[
\rho_i = \sum_{j=0}^{\rho_i} \rho_j(\mathbf{r}_i)
\]

\( \rho_i \) is the sum of the individual electron density provided by the other atoms of the system, \( F_i(\rho_i) \) is the energy needed to integrate the atom i into the local electronic charge density, \( \phi_{ij}(r_{ij}) \) is a pairwise electrostatic interaction between atom i and atom j separated by distance \( \mathbf{r}_{ij} \) and \( \rho_j \) is the electron density provided by the atom j.

Here, we focused our attention on the diffusion of two islands of type \( \text{Au}_4 \) (tetramers) on \( \text{Ag}(110) \) surface \( \text{Au}_4\)/Ag(110). The motivation of this study is to reveal the atomic processes responsible for the diffusion of the clusters and their coalescences. This study is performed through using molecular dynamics. Simulations were performed for a two-sided free surface substrate containing 5400 atoms for a six-layer symmetry (110) having (30 x 30) atoms in each layer. Here, the x and y axes are located in the plane of the surface, while the z axis is perpendicular to the surface. In the surface plane, the periodic boundary conditions have been made along the x and y directions, but not in the z direction, to ensure the deposition of adatoms. Optimization of the geometry is performed at 0K by minimizing their energy and then relaxing the system for 40 \( \mu \)s under the micro-canonical conditions, as shown in the following diagram :
Fig. 1. Representation of the substrate construction contains three areas: free region (2 layers at the top); Isothermal region (2 layers in the middle) fixed region (2 layers down).

This part was the subject of an investigation on the dynamics of the two islands (tetramers) on a substrate of an orientation (110), and this for different forms (4S-4S, 4T-4T, 4N-4N) and positions as well as separation distances Fig.2. The study in question was developed in a temperature range from 300K to 700K.

Fig. 2. Representation of the different structures of the system: (a) two square islands separated by n site following the channel (IC) SSn, (b) two separate square islands by n site through the channel (CC) SSn, (c) two islands of form T separated by n site along the channel (IC) TTn (d) two islands of N form separated by n site following the channel (IC) NNn . (N = 1, 2)

3. Results and discussion

In what follows, we will scroll through all the results obtained during the static and dynamic study of the coalescence of two tetramers islands Au₄ / Au₄ / Ag(110) for temperatures ranging from 300K up to 700K.

3.1 Static study

In the first place, a study was made on the removal of an adatom attached to an island which can take several sizes from 2 to 16 atoms; our investigation also focused on the influence of island size on the displacement of the torn adatom for the systems (Au / Ag, Cu / Ag, Pt / Ag) at 300K.

Fig. 3b, which represents the displacement of an adatom attached to islands of different sizes with respect to the substrate adsorption site. It shows that the Au adatom has a mismatch of the order of 0.24% <1% [44], experienced a shift of 0.11 Å for the sizes of islands of less than 6 atoms, after this shift, the displacement increases with the enlargement of the islands size up to a value of 0.15 Å, beyond the islands a size of 12 atoms this shift is stabilized. However, for the two Pt / Ag and Cu / Ag
systems that have an incoherent mesh mismatch greater than 1%, the adatom displacement attached to the 2 to 12 atom size islands increases. In a linear fashion from 0.23 to 0.35 Å, beyond a block size greater than 12 adatoms the displacement recognized a small increase to a value of 0.36Å. Thus, the cleavage between the adatoms and the substrate produces a displacement of the adatoms relative to the absorption site; this displacement increases with the increase of disagreement for a size of an island less than 12 atoms. However, in the opposite case when the adatoms have larger sizes compared to that of the substrate, the displacement of the adatoms increases as well and when the sizes of the islands [48].

Figure 3 (a) shows the detachment energy of an adatom at a cluster as a function of island size. It is shown that the energy of the Au / Ag system decreases exponentially with the increase of the size of the islands up to the size of 12 adatoms, after which it stabilizes towards a value of 0.255 eV, while the two other systems Pt / Ag and Cu / Ag have known values between 0.235 and 0.22 eV depending on the number of adatoms constituting these islands. By analogy, from the representation of the displacement of adatom as a function of the size of the islands, Figure 3 (b) gives the same description to the atomic tearing energies for the three systems as a function of the size of the system.

Figure 4 (a) shows the study of the formation energy as a function of the number of separation sites for two tetramers of SS (IC) and SS (CC) form; it is seen that for these two forms of SS, the formation energy is very important for the case of two adjacent islands of in-channel SS (IC) and which are 1.76 eV compared to the case cross-channel SS (CC) which is 1.55 eV. After a separation site, the formation energies coincide in the same values that are close to 1.26 eV fig.4a. On the other hand, for both forms of the TT and NN in-channel (IC) system, the process is reversed. The same energy value is found for the case of two adjacent islands having a value of 1.75 eV, which is explained by the same basic geometry of these two forms. After a separation site, in each case, the formation energy tends to a value of 1.17 eV for TT and 1.24 eV for the form NN. Therefore, the separation of the islands beyond an adsorption site gives a formation energy value depending on the geometric shape of these islands.
3.2 Dynamic study

In this part, we will focus our attention on the dynamic evolution of the two islands (tetramers) of system Ag$_4$/Ag(110), during a duration of 10ns at different temperatures included between 300K and 700K. This study focused on the forms of the cited systems, namely SS (IC), (CC) as well as TT and NN (IC). It is noted that in the range of 300K to 450K the islands of forms SS remains stable along the dynamic evolution, unlike other forms, from where the diffusion is triggered from 400 K, which explains the instability of TT and NN shapes compared to the SS form [26] [49].

Figures 5-8 show the evolution of SS-type islands at different temperatures, summarizing the set of possible training mechanisms for this configuration.

Fig. 5 represents two SS-in-Channel (IC) shaped islands at a temperature of 550 K. The connection was made by the migration of the two atoms from one island to the other successively along the channel fig. 5b-c, thereafter the third atom makes an exchange with an atom of the substrate which belongs to the channel on which the large islet is adsorbed, in order to facilitate the grouping by simple diffusion mechanisms, arriving at a partial homogeneous coalescence (islet) of 6 adatoms). However, for the temperatures of 600K and 650K, the exchange mechanisms become priority to make the connections between the islands in order to have a total heterogeneous coalescence.

Figure 6 shows that the two islands of SS system at a temperature of 550 K started with a connection between them through a mechanism of exchange of a dimer (fig. 6b) with the evolution in time this system forms an island with six heterogeneous atoms by two mechanisms of exchange and diffusion of a dimer fig. 6c-d.

Fig. 4. the formation energy according to the positions.
Fig. 6. Dynamic evolution of two islands of an SS cross Channel form at 550 K.

In fig. 7, two islands having an SS cross-Channel shape at the connected temperature of 600 K are represented. This result shows that two atoms belonging to the same island making an exchange mechanism with two atoms of the substrate forming part of the channel on which the other island is adsorbed. In order to facilitate the grouping by simple diffusion mechanisms fig. 7b. Thus, the coalescence between the 2 islands SS (CC) begins with the mechanisms exchange with the atoms of the channel on which is adsorbed, falling in continuation in the mechanisms of coalescence in the case of SS (IC) systems.

Fig. 7. Dynamic evolution of two islands for SS cross channel form at 600 K.

The results of fig. 8 represent the evolution of the SS1-SS1 (IC) structure at 650K. The coalescence between the two islands is done through a multitude of exchange-jump processes in order to arrive at a heterogeneous island of 8 adatoms (figs. (B), (c) and (d))
Fig. 8. Dynamic evolution of two islands of an SS in Channel form at 650 K.

Figures 9-10 show the evolution of NN and TT type islands at different temperatures, summarizing the set of possible training mechanisms for this configuration. Fig. 9 shows that at a temperature of 500K, the NN islands undergo an exchange, which gives a total heterogeneous coalescence fig.9, b, the evolution over time makes it possible to arrive at an island comprising nine heterogeneous atoms across the planet. Attachment of an adatome fig. 9c-d, for a temperature of 600K, we see that a total heterogeneous coalescence has taken place, with the construction of an island of eight atoms through mechanisms of jumps and exchanges (fig. 10 b-c-d).

Fig. 9. Dynamic evolution of two islets for NN in channel form at 500 K

Fig. 10. Dynamic evolution of two islands for NN in channel form at 600 K.
Figures 11: b-c shows that at a temperature of 450K each one of two islands T attached to one adatom of the other island T to give a single island formed by two linear tetramers (the most stable form), we can say that we have a homogeneous total coalescence. The evolution of the temperature towards 600K makes it possible to distinguish almost the same behavior with the appearance of a homogeneous partial coalescence; whereas, for 550K fig. 12, through the same diffusion processes the TT form tends towards a heterogeneous partial coalescence fig. 12 c, but over time the island changes its structure fig.12 d.

![Fig. 11. Dynamic evolution of two islands for TT in channel form at 450 K.](image1)

Fig. 12. Dynamic evolution of two islands for TT in channel form at 550 K.

Fig. 13 (a) shows the evolution of the lifetime of the system of two islands of SS type deposited in-Channel as a function of temperature, the corresponding results showing that the system SS1 diffuses from the temperature 400K; however, both SS2 and SS3 systems withstand a temperature of 450K. However, during the increase of the temperature a decrease in the life of the system is observed, beyond 600K the three systems have a very short life (<20 ps).

The results of fig. 13 (b) show the evolution of the time of coalescence of the two-island SS type system deposited in-Channel as a function of temperature. This appearance shows that the three systems SS1, SS2 and SS3 obey successively coalescing at 400K, 450K and 500K. As the temperature increases, the time of coalescence decreases significantly; but beyond 600K, the coalescence time of the three systems becomes fast, which is reflected by a decrease in the slope of variation of the service life with respect to the temperature.
Fig. 13. (a) Represents the system life of two islets (SS) as a function of temperature, (b) Represents the time of the appearance of coalescence of two islands (S) as a function of temperature for the system in cross-channel.

In the case where the two SS islands are deposited in cross-Channel, fig. 14 (a), describes the evolution of the life of this form as a function of temperature. It shows that from a temperature of 400K SS1 system diffuses for a very short time, against both systems SS2 and SS3 withstands a temperature of 450K, as the temperature increases the duration of life decreases after 600K the three systems coalesce quickly.

Figure: 14 (b) represents the evolution of the coalescence time of the system of two islands of SS type deposited in-Channel as a function of the temperature; it is observed that from 500K the three systems SS1, SS2 and SS3 obey a coalescence. As the temperature increases, there is a decrease in the time when diffusion processes occur to coalesce the two islands.

Fig. 14. (a) Represents the system life of two islets (SS) as a function of temperature, (b) Represents the time of the appearance of coalescence of two islands (S) as a function of temperature for the system in channel.

Figure: 15 (a) shows the evolution of the service life of the two TT-in-Channel island systems as a function of temperature, it is shown that from a temperature of 400K, the three TT1 systems, TT2 and TT3 diffuse by a sudden fall simultaneously during the increase of temperature, beyond 550K the systems its moments of coalescence becomes small (<60 ps). Fig. 15 (b) shows the evolution of the coalescence time of the two TT-in-Channel island system as a function of temperature. Note that from 400K the three systems TT1, TT2 and TT3 obey a coalescence during an increase in temperature, there is then a decrease in the duration of coalescence.
Fig. 15. (a) Represents the system life of two islets (TT) as a function of temperature, (b) Represents the time of the appearance of coalescence of two islands (TT) as a function of temperature for the system Au_{110} / Ag(110) in channel.

Figure 16 (a) shows the evolution of the lifetime of the system of two TT-in-Channel islands as a function of temperature, it is shown that starting from a temperature of 400K the three NN1 systems, NN2 and NN3 are spread by a sudden simultaneous fall. During the increase of the temperature, and beyond 550K the systems its moments of coalescence become smaller (<60 ps).

Figure 16 (b) represents the evolution of the time of the coalescence of the system of two islands of NN type in-Channel as a function of the temperature, we note that from 400K the three systems NN1, NN2 and NN3 obey to a coalescence. It is obvious that when the temperature increases a decrease in the duration of the coalescence is observed.

Figures 17-18 illustrates a comparison of the duration of diffusion / coalescence versus temperature for the four subject systems of our investigation. It has been shown that for the SS (IC) system, at the presence of a single SS1 separation site, the scattering is triggered at a very high rate at 450K by sweeping a duration of 3800 ps between diffusion and coalescence, the latter decreasing by increasing the temperature, marking periods more or less short since 600K. For both systems SS2 and SS3, the diffusion starts at 500K with different duration of the diffusion until the coalescence having values 2800 and 5700 ps respectively (fig.17-a).

As regards, the Cross-Channel (CC) process for the SS form, it can be seen that, in the presence of two separation sites SS2, the diffusion starts at a temperature of 450K with a diffusion / coalescence duration of 9300 ps. This duration decreases gradually as the temperature increases. For both SS1 and SS3 systems, the periods required to reach coalescence after diffusion are 6900 and 7800 Ps respectively. In the same way, this duration decreases by increasing the temperature (fig.17-b)
Fig. 17. (a) Represents the diffusion time of the two island system (SS (IC)) as a function of temperature, (b) Represents the diffusion time of the two island system (SS (CC)) as a function of temperature, for the system Au$_4$/Ag(110).

In the TT and NN form systems (fig. 18a-b), diffusion occurs at a temperature of 450K for the three separation sites TT$n$ and NN$n$ with $n = 1, 2$ and 3. The diffusion / coalescence time is included in the range 3600-4700 ps for the form TT$n$, as for the form NN$n$ said duration diffusion / coalescence, fits in the range 2400-4700 ps. This duration decreases by increasing the temperature and marks very small values (<90 ps) beyond 600K.

Fig. 18. (a) Represents the diffusion time of the two island system (TT (IC)) as a function of temperature, (b) Represents the diffusion time of the two island system (NN (IC)) as a function of temperature, for the system Au$_4$/Ag(110).

It can be concluded, then, that the temperature has a remarkable effect on the duration of diffusion / coalescence. The increase in temperature causes a decrease in the duration in question which intensifies beyond 600K and this for all systems studied. A slightly moderate decrease between 450 and 600K explains the good activity of the coalescence of islands in this temperature range.

4. Conclusion

In the present work, we studied by the molecular dynamics method, the coalescence of two tetrameric islands of the three forms SS, TT and NN. These islands are deposited at different spacings following and through the channel in a temperature range from 300K to 700K. From the results obtained, it can be concluded that the detachment energy of an adatom of a cluster is decreased by increasing the size of the island. Thus, the adatom displacement attached to islands of varying size from 2 to 12 adatoms increases proportionally with its size in a way that reduces the spacing between the island and the attachment adatom producing an island restriction. It is noted that the separation of islands beyond an absorption site gives a value of formation energy constant and dependent on the geometric shape of these islands. This dynamic study shows that at low temperature (<400K for TT, NN (IC) and <450K for SS (IC), SS (CC)) the system remains stable. On the other hand, in the
temperature range between 450 and 650 K, one meets the phenomenology of the homogeneous partial coalescence induced by mechanisms of jumps, thus, the increase of the temperature in this interval favors the mechanisms of exchange which generates a coalescence total heterogeneous.

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