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Surface diffusion and cluster formation of gold on the silicon (111)

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ABSTRACT

Purpose: Investigation of the gold atoms behaviour on the surface of silicon by molecular dynamics simulation method. The studies were performed for the case of one, two and four atoms, as well as incomplete and complete filling of gold atoms on the silicon surface.

Design/methodology/approach: Investigations were performed by the method of molecular dynamics simulation using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). MEAM potential of interatomic interaction was used for modelling. Molecular dynamic simulations were carried out in isothermal-isobaric ensemble (NpT) with a timestep 1.0 fs.

Findings: As a result of studies, the preferred interaction between gold atoms and the formation of clusters at temperatures up to 800 K was revealed. Analysis of the temperature dependences of the number of large jumps of atoms made it possible to calculate the activation energy of a single jump. It was found that activation energy of single atomic displacement decreases with increasing number of gold atoms.

Research limitations/implications: Only a limited number of sets of atoms were used in the study. It is possible that for another combination of atoms and a larger substrate surface, the formation of gold nanoislands on the silicon surface can be observed, which requires further research.

Practical implications: The research results can be used to select the modes of gold sputtering to create gold nanoislands or nanopillars on the silicon surface.

Originality/value: Computer modelling of the behaviour of gold atoms on the surface of silicon with the possibility of their self-organization and cluster formation was performed for the first time.

Keywords: Molecular dynamics, Surface diffusion, Clusters, Atomic monolayer, Activation energy

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MATERIALS

1. Introduction

Investigations of material properties in the nanoscale become major topic from the fundamental and applied point of view. The properties of such materials, are highly sensitive not only to the size, but also to the shape and composition of the atomic clusters or precipitates [1-3]. As it is known, the methods of obtaining nanoparticles are divided into two classes, namely, bottom-up approach or the top-down one. Interpretation of the motion of single atom or group of atoms are becoming quite an interesting task for the bottom-up approach. During the change of cluster size from an isolated atom to a bulk phase, the peculiar properties change as the function of the size of such cluster. To achieve potential industrial applications of nanoparticles and nanosystems, investigation of atomic motions is needed for the case of one and several adatoms on a given substrate surface in order to understand the mechanism of nanoparticle formation process [4]. Moreover the understanding of cluster formation processes is very important for studying of self-organization phenomena at nonequilibrium conditions. On that reason the controlled self-assembly of gold nanoparticles on crystal silicon surfaces, studied in this work, which is one of the problems of great interest and is one of steps to make more completed the knowledge about such science as synergetics.

In nanometre scale, gold particles often exhibit unique electronic, magnetic, photonic and catalytic properties [5,6]. Results of experimental and Molecular Dynamics (MD) investigations allow us to complement the theory of the gold nanostructures formation. Such theory can be then used to fabricate novel and larger integrated devices.

There is a lot of methods to produce gold nanoparticles, where nanoislands of gold are formed on crystal silicon or other (e.g. carbon or graphene) substrates [7,8]. Initially, these structures are often created by atom-by-atom coating methods. This means, that at the first steps of such processes, system in the form of isolated gold atom on a chosen substrate is created. In view of this, the question arises about how atom behaves on a free surface, for example, how its random movements can lead to the formation of a cluster? What relationship exists between particles relaxation kinetics and temperature? The main goal of this work is to shed light on the aforementioned issues. The growth mechanism of gold nanoislands on silicon surface is thought to involve diffusion and interdiffusion processes with additional eutectic alloy formation. A wide range of experimental works have already tried to explain these processes. The most prominent works are those which for example confirm initially proposed theories such as Volmer-Weber [9] theory or the classical Burton-Cabrera-Frank theory [10]. On the other hand, there are investigations which have concluded that the coalescence processes or the mechanism of Ostwald ripening are the main drives behind the formation of gold nanoislands. For a deeper analysis of the processes described in this works, diffusion processes have also been studied by use of Molecular Dynamics simulations.

Due to the fact that experimental techiniques are often difficult and expensive to apply for macro scale and atomic level investigations of bulk and surface properties, numerical analysis and computer simulation methods can be used to obtain reliable results [11-14]. These works highlight the results of investigations at various spatial levels - from the macro level to the atomic level and show the full power of computational methods in materials science. In particular, Ref. [12] presents the results of optimization of structural elements working in the environment of cavitation wear together with a computer numerical analysis at the macrolevel. At the micro level, for example, it is possible to model the casting process and the microstructure of cast steels [11]. Review article [13] analyses the possibility of using the finite element method for simulation 2D objects, namely to determine the properties of PVD and CVD coatings on various substrates. Finally, in [14] the study of diffusion processes at the gold-silicon boundary by the method of modular dynamics at the atomic level was carried out.

It has been also confirmed experimentally [15], theoretically [16], and using the aforementioned MD method, that diffusion of individual particles during the formation of gold clusters are quite comparable to the rates exhibited by single atoms systems in similar conditions. This means that results obtained by investigating diffusion of one atom on a crystal silicon surface via MD method can be used to properly describe the movement of atom in case of gold nanoislands formation. Therefore, computational methods constitute a much less expensive alternative to experimental ones and still allow us to achieve physical results.

In our work, we examine the nature of mass transport mechanisms during the fundamental phase transition processes i.e. during the vapour-liquid-solid transition of gold nanocoatings on crystal silicon surface. This investigation is carried out for systems ranging from single gold ad-atom system up to the system where a whole monolayer of gold is deposited upon Si(111) substrate. The system Au-Si(111) was chosen due to the fact that it has long been a prototype system for metal-semiconductor interactions and Si(111) shows a rich variety of surface reconstructions upon metal adsorption. For Au on Si(111), different surface reconstructions have been identified at various elevated temperatures.

The expected result is to observe the migration of gold atoms starting with individual isolated particles to aforementioned clusters. This was done for a range of different temperatures to also check how the change of thermodynamic conditions affects the random movement of atoms within considered systems.

2. Computational details

Molecular dynamics simulations in this work were performed by using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [17]. To create simulation systems, we started with a silicon surface created from a bulk silicon substrate of dimensions 32.5, 32.5, 48.8 Å along x, y and z-axis respectively. The crystallographic direction was set to x [1 0 0], y [0 1 0], z [0 0 1]. This bulk substrate consisted of 2664 Si atoms. Si atoms from the bottom layer, with a thickness of 20.4 Å, were frozen to mimic the semi-infinite surface. MD simulations were carried out in isothermal-isobaric ensemble (NpT) with a timestep 1.0 fs. Simulations were carried out for the temperature range from 525 K to 925 K, with a step of 50 K set between each of them. The initialization of velocities was carried out using Maxwell-Boltzmann distribution. In the beginning, each system in the form of an orthogonal simulation box has been equilibrated for 200 000 timesteps. The damping parameter for temperature has been set to 100 timesteps and for pressure damping - 1000 timesteps. After the initial equilibration, the duration of the sampling part of simulations was set to 51000 timesteps. In the case of systems containing more than one gold adatom this period has been extended to 500 000 timesteps. During calculations, periodic boundary conditions (PBC) were employed only in two Cartesian directions, excluding the z-axis. Spatial configurations of each of the consecutive timesteps were written to an external data file. For the isolated Au adatoms on the substrate, an energy minimization has also been performed before the equilibration stage, which allowed achieving an equilibrium state during further parts of the simulation more quickly. The system was extended to 200 Å along the z-axis to create a free space above the gold ad-atoms. This was done in accordance with the experimental conditions used during the fabrication of such systems, where before deposition of the atoms, the surface is kept under vacuum conditions.

The Au-Si interatomic interaction has been modelled using a version of MEAM potential parameterized by Ryu and Cai [18]. In the MEAM formalism, the potential energy functional can be expressed as

$$V(r_i) = \sum_{i=1}^{N} F(\bar{\rho}_i) + \sum_{i=0}^{N-1} \sum_{j=i+1}^{N} S_{ij}\phi_{ij}\left(|r_i - r_j|\right), \quad (1)$$

where F is the embedding function, $\bar{\rho}_i$ is the background electron density at r_i, S_{ij} is a multi-body screening factor and ϕ_{ij} is the pair potential of atoms i and j.

3. Results and discussion

For single Au atom systems, the results are as follows. Most of the displacements of Au ad-atom were smaller than the diameter of the silicon atom(2,22 Å), which means that they were thermal oscillations around Si lattice sites. The initial position of Au atom was (12.219, 12.219, 51.203 Å), after the energy minimization stage Figure 1(a).

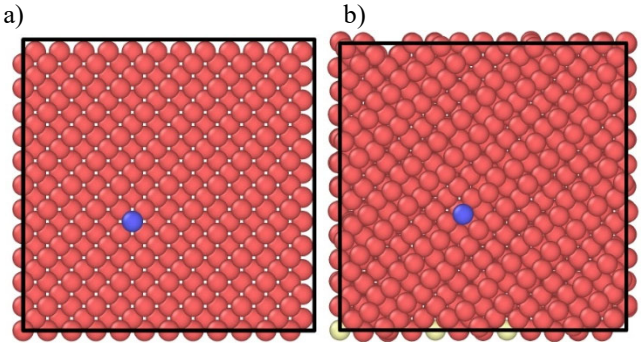

Fig. 1. Visualization of the single Au adatom system in its initial (a) and final (b) state for simulation carried out in the temperature of 575 K

At temperature 575 K, the gold atom oscillated at the crystalline silicon surface i.e. it did not travel long distances with respect to its initial position Figure 1(b).

Due to the raise of the temperature, the mobility of Si has visibly increased. This in turn created additional paths of gold atom migration on the surface of silicon. At the same time, there was a reduction in the neighbouring positions that it could jump over to. This caused the displacements to be at further distances from the initial position of the gold atom. The main mechanism of these jumps was random walk and interstitial diffusion.

Characterization of the behaviour of single gold atom displacements at different temperatures was done by analysing Mean Square Displacement (MSD) and random walk figures. We have separated 4 individual displacement types for the entire temperature range. As you can see, at 575 K the gold atom has made several jumps Figures 2(a,b),

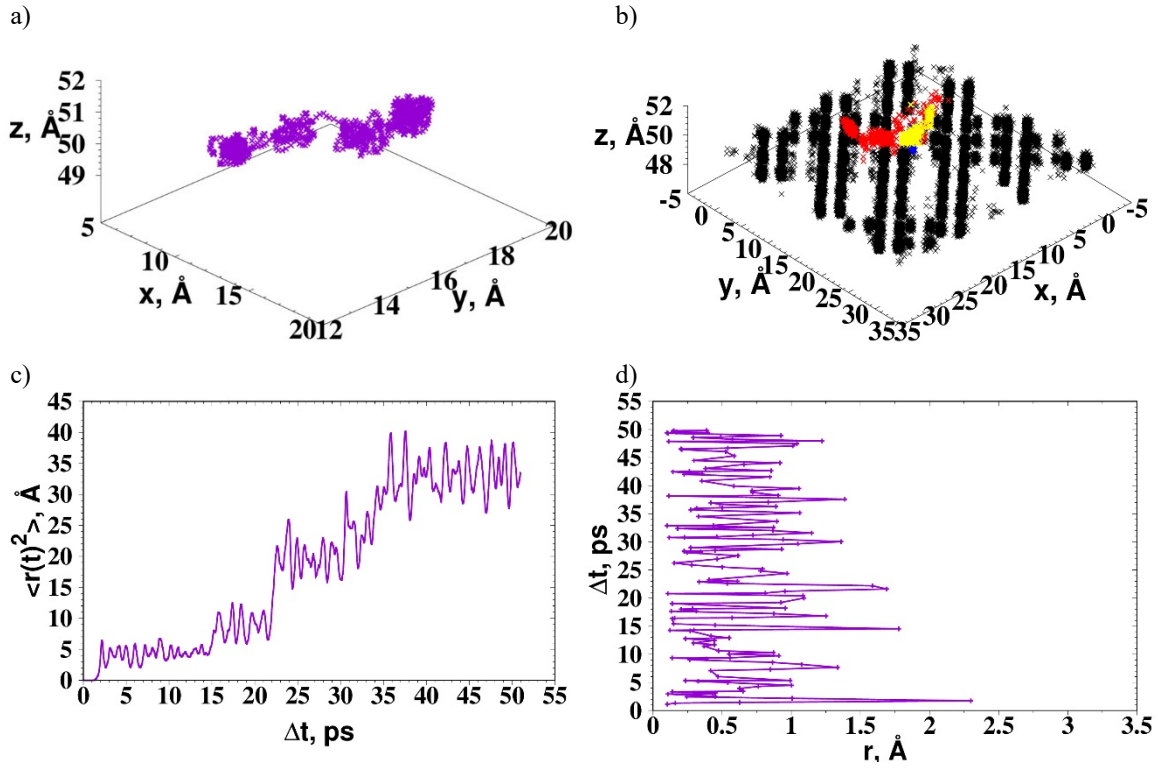

Fig. 2. Representation of Au-atom displacement at 575 K a), b) random walk of Au particle; c) mean square displacement; d) length of each individual jump

where after each of them it proceeded to oscillate at the subsequent interstitial positions. This is further shown by the MSD charts Figure 2(c). Most frequent behaviour was observed for 625, 725, 775, 825, 975, 1025 and consists of only two jumps, as shown at Figure 3 for 625 K. Next one is a pattern of three single jumps, which is visible in case of temperatures equal to 675, 875 and 925 K. This type of random walk is presented in Figure 4. For 575 K we do not have the same behaviour as described above i.e. the random walk in this case consists of 4 single jumps and quite long-time oscillations in equilibrium positions. Figure 2(c) shows the individual jumps registered during the simulation. As you can see, most of these jumps are of small distances, not exceeding 75% Si atomic diameter i.e. the value of 2.16 Å. During the jump the direction of the gold atom displacement changes after collision with Si atoms. To investigate this behaviour, the length of each individual jump was calculated Figure 2(d). During the simulation, a surface diffusion has been observed. At high temperatures, the gold atom may also move into the first or second silicon atomic planes.

MSD show that at the temperatures close to 675 K, the gold atom has more variation to its displacements. In these subsequent positions, the atom continues to oscillate, before making another transition.

When the temperature increases, the number of preferable jump positions is smaller, which makes the jumps take place at smaller distances. The phenomenon often observed during simulations is that the gold atom returns to the previous location after a series of continuous jumps. One explanation is the dynamic nature of the atomic reorganization, which takes place before the phase transition of the silicon substrate.

Temperature dependence of parameters such as the average jump distance, the average jump time, the maximum distance to which a single atom skips and the number of jumps registered during simulations are shown in Figures 5 and 6.

For the calculation of numbers and distances of jumps, the numerical behaviour of this parameters were analysed. It was noticed that the subsequent coordinates of the gold atom jump have monotone behaviour – they either increase. Due to the fact that the gold atom is on the silicon surface, a displacement equal to 75% of Si atomic diameter was considered to be a jump. It was revealed that the amplitude of gold atom thermal oscillations was always below this value. The graphs show almost linear dependences, with exclusion of the several sampling points. The main force of motion is thermal excitation.

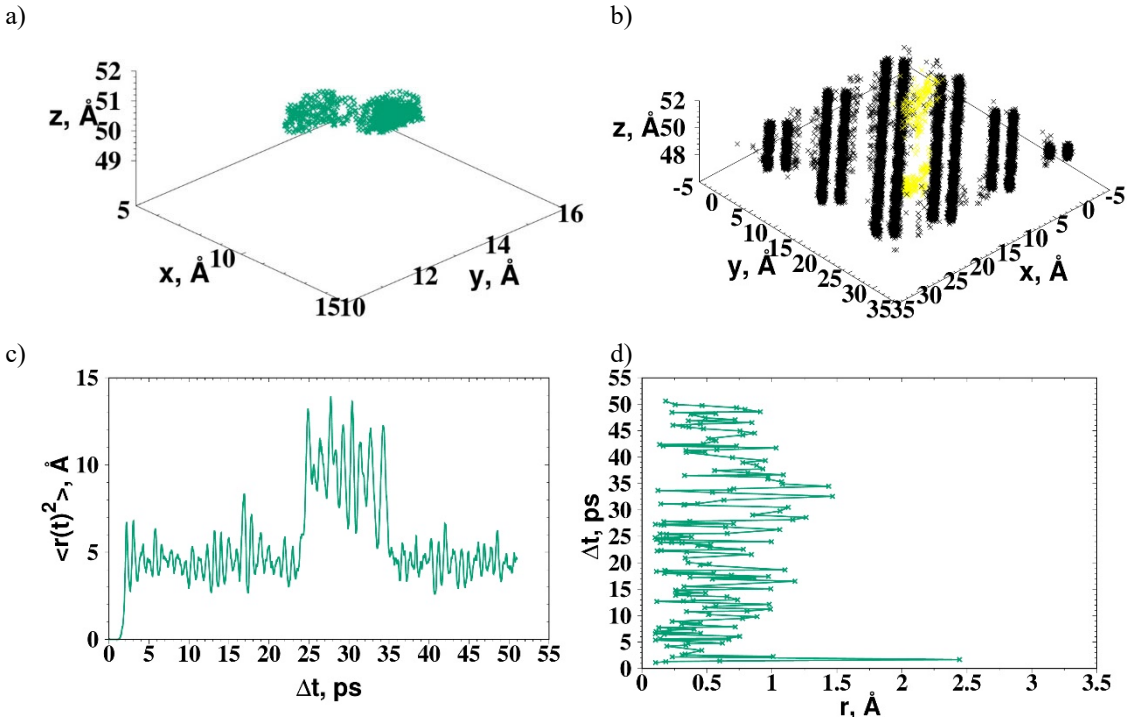

Fig. 3. Representation of Au-atom displacement at 625 K a),b) random walk of Au particle; c) mean square displacement; d) length of each individual jump

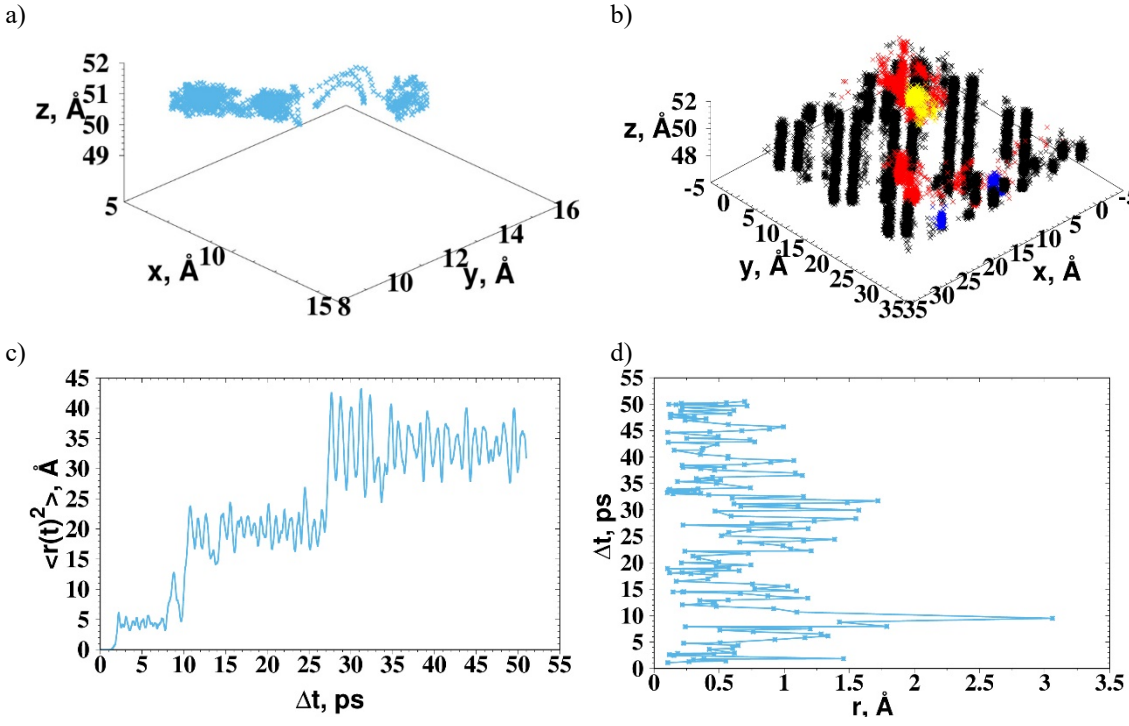

Fig. 4. Representation of Au-atom displacement at 675 K a), b) random walk of Au particle; c) mean square displacement; d) length of each individual jump

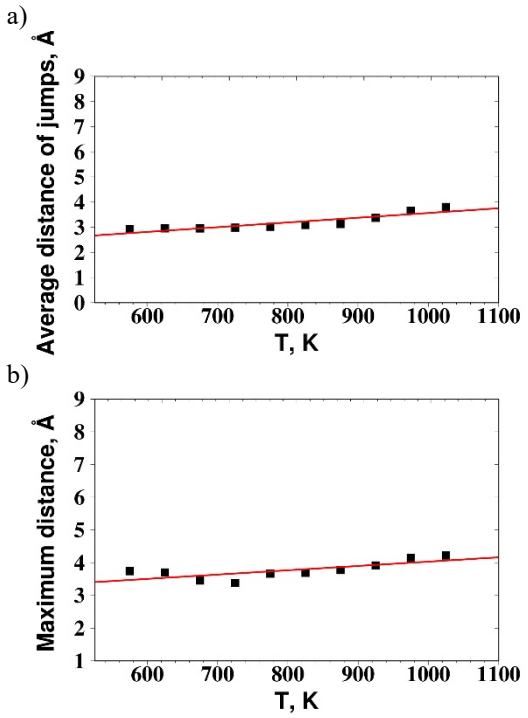

Fig. 5. Temperature dependence of displacement distances: a) average distance of jumps, b) maximum distance of jumps

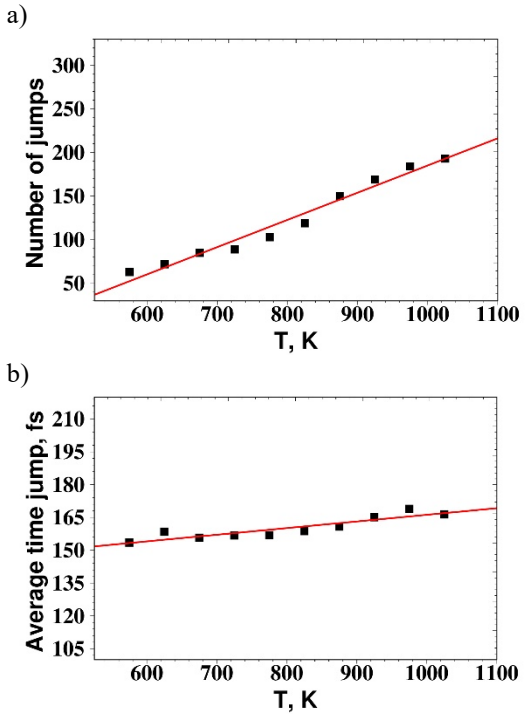

Fig. 6. Temperature dependence of number (a) and time (b) of jumps

In the next stage, we examined the displacements of two gold atoms that are close to each other. At the beginning of the simulation, the gold atoms were connected into pairs. At a temperature close to 675 K, the pair of Au atoms travels together at short distances. As the temperature increases, the pair of gold atoms has fewer preferable jump positions, because the size of the atomic pair is larger than a single atom. In case of the temperature distortion of the silicon substrate, observed at the end of the simulation, the system of two atoms did not move far from the initial position, instead oscillating in their original position. As in the case of one gold atom, the surface diffusion also occurs. This type of atomic displacement is observed in a wide temperature range (Fig. 7). Only at the temperature equal to 925 K Figure 8, the interaction between atoms decreases and they move independently of each other.

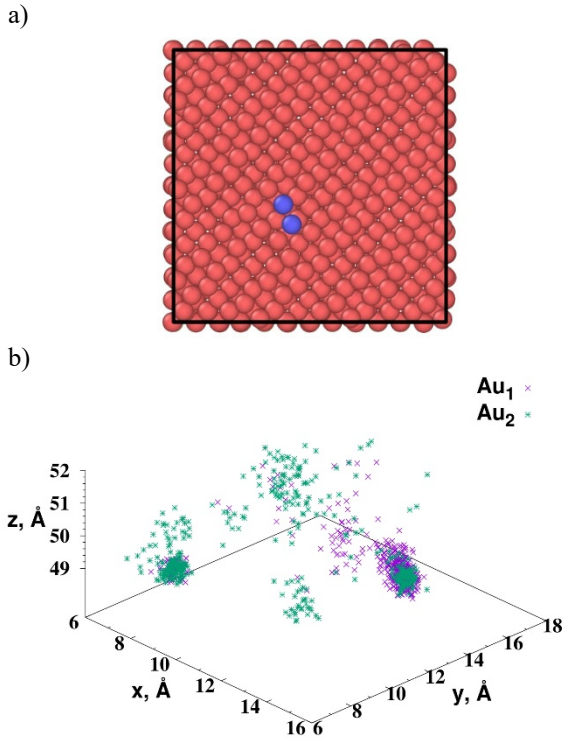

Fig. 7. Visualization of the atomic pair system simulations carried out at the temperature of 675 K

For a system with 4 atoms, the situation is similar to a pair of atoms at low temperatures. Due to the fact that this type of systems results in gold atoms connected into a cluster, the visualization of their random walk is more difficult. This can be seen in the snapshots presented at Figure 9. In this case, we have used figures generated by The Open Visualization Tool (OVITO) [19].

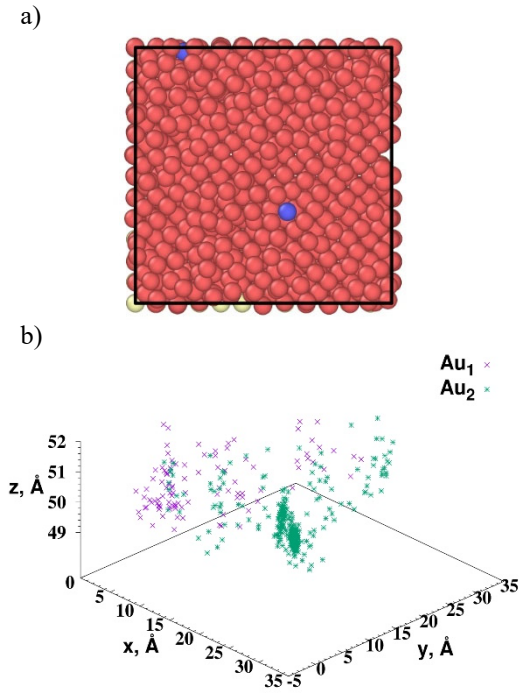

Fig. 8. Visualization of the atomic pair system simulations carried out at the temperature of 925 K

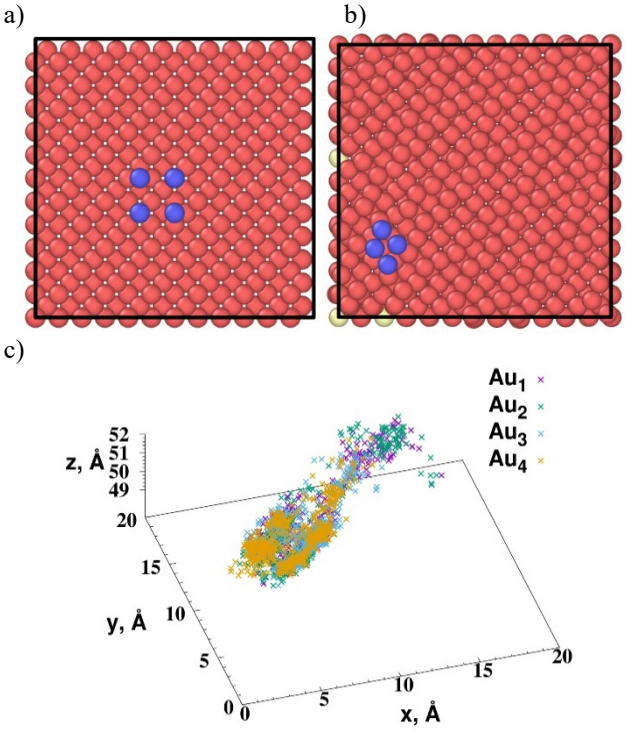

Fig. 9. Visualization of the 4 atom cluster system in its initial (a) and final (b) state for simulation carried out in the temperature of 575 K (c)

The analysis identified three possible mechanisms. The first is that each individual atom performs a certain number of jumps and connected into a cluster. The second when only 3 out of 4 gold atoms form a cluster, seen for example at a temperature of 725 K Figure 10(a). The third case is observed when during large oscillations of the silicon substrate, the four atoms disconnect completely from each other and the cluster is not formed. This behaviour has been observed e.g. at temperature of 925 K Figure 10(b). After analysing the movement and oscillations, we presented the basic mechanism for forming larger clusters.

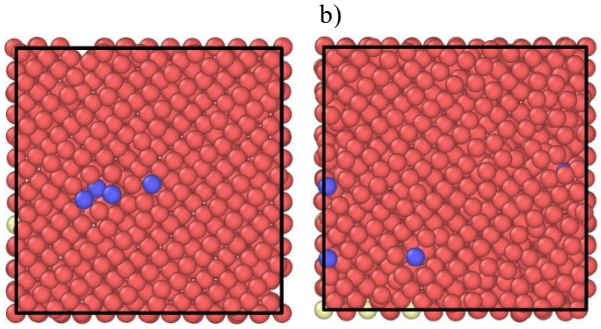

Fig. 10. Visualization of the 4 atom cluster system in its final state for simulation: a) 725 K, b) 925 K

The results of the behaviour of isolated atoms on the silicon surface obtained by us are consistent with the similar behaviour of atoms on the graphite surface studied by experimental methods [20]. In this paper it is indicated that in the case of one atom it moves short distances, remaining near a local region. If there are two atoms on the carbon surface, they display obvious interaction behaviour. In this case, the formation of dimers occurs. Atomic dimers rotate on the carbon substrate, the dimer separates into two isolated atoms, and finally it reassembles into another dimer. Similar behaviour of two atoms is observed in our studies.

Described above results were obtained for connected Au atoms before simulations. On the next step, simulations were carried out for 64 gold atoms that were randomly located on a silicon substrate Figure 11(a). In this case, the gold atoms fill half of the monolayer (0.5 ML) on the silicon surface.

It can be seen that gold atoms at the temperature close to 675 K form small groups Figure 11(b), near the positions of the largest concentration of gold particles. At 725 K Figures 12(a), and 12(b), the formation of groups with surface diffusion taking place is also visible. However, the clusters may lose individual atoms or pairs of atoms over time.

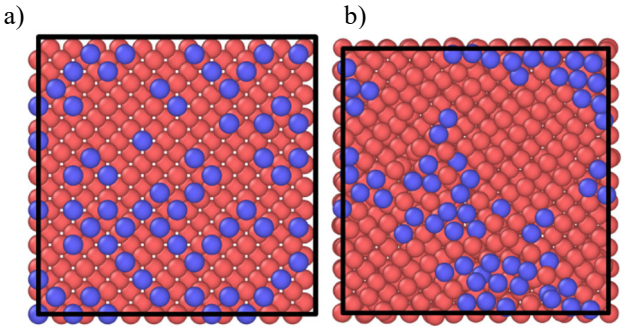

Fig. 11. Visualization of the 50% Au atoms of 1 ML system in its initial (a) and final (b) state for simulation carried out in the temperature of 575 K

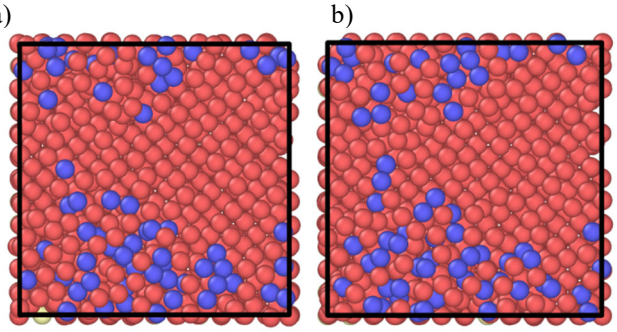

Fig. 12. Visualization of the 50% Au atoms of 1 ML system in its middle (a) and final (b) timestep state for simulation carried out in the temperature of 725 K

For quantitative analysis of the surface diffusion process of gold atoms on the silicon surface, the temperature dependences of the average distances (Fig. 13 a) between the gold atoms and the activation energy of a single jump (Fig. 13b) were calculated. Activation energy was calculated from the analysis of Arrhenius plots (Fig. 14).

Analysis of the temperature dependences of the average interatomic distances indicates that the temperature stability of gold clusters decreases with decreasing number of atoms in the cluster. This is indicated by the sharp increase in interatomic distances with increasing temperature for the case of a small number of gold atoms. Nevertheless, the activation energy of the single atom jump increases with the decrease in the number of atoms and for the case of one atom on the silicon surface is 1.7 eV (Fig. 13b).

The results obtained above made it possible to understand the behaviour of a small number of gold atoms on the silicon surface. For the subsequent simulations, we used a two times wider system, which had 9440 of all atoms and 512 gold atoms (Fig. 15).

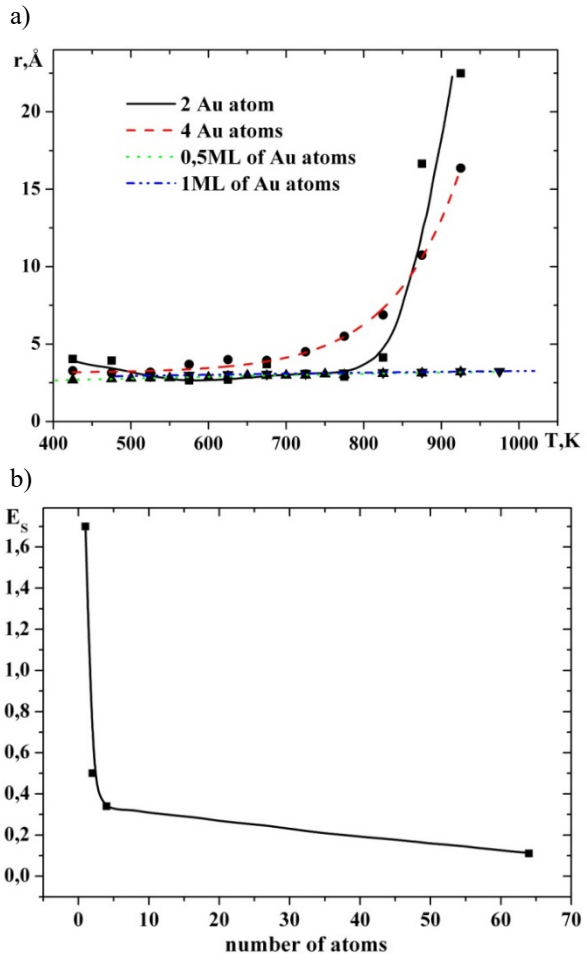

Fig. 13. Temperature dependence of mean interatomic distances (a) and activation energy of a single atomic jump (b)

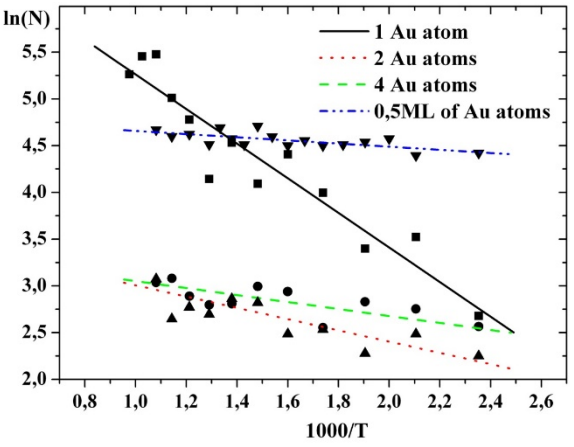

Fig. 14. Dependence of the number of single jumps of the Au-atoms on the Si surface versus inverse temperature

The next step was to locate Au atoms at greater distances from each other to exclude the possibility of joining them in the above mentioned groups. This atoms are about 13% of monolayer Fig. 15(a). The simulation results are similar to the aforementioned cases, i.e. the attraction of gold particles is observed, which in the future may be the beginning of the creation of centres for nanoscale gold clusters on a macroscopic level.

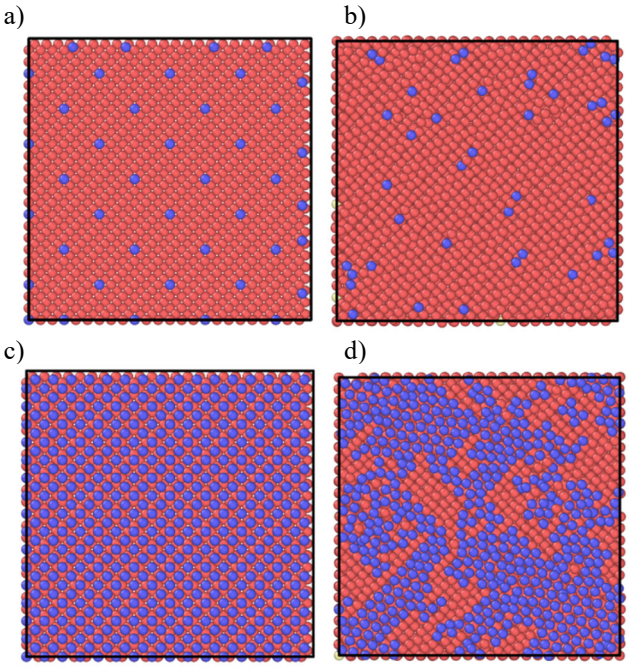

Fig. 15. Visualization of 13% Au atoms (upper panel) and 1 ML system (lower panel) in its initial (a, c) and final (b, d) state for simulation carried out in the temperature of 525 K

The simulation of a single monolayer of gold atoms on the silicon surface is consistent with the results obtained for a smaller number of atoms. In particular, the preferred interaction between the gold atoms is observed resulting in their clustering. As can be seen from Figure 15(d), the boundaries of the clusters are oriented along the silicon atomic series, that is, along the channels of simpler atomic displacement. At higher temperatures (Fig. 16), the clustering of atoms is also observed, but the outlines of the clusters become less clear. In this case, it should also be noted that for the case of one monolayer of gold on the silicon surface, the temperature dependence of the number of Au atoms jumps which commensurate with the size of the silicon atom differs from the cases described above. For a small number of atoms, the number of large jumps of gold atoms increases with temperature. In the case of one entire monolayer of gold atoms on silicon, the number of large jumps decreases with increasing temperature. The reason for this is obviously the significant interaction between the atoms of gold and silicon, as a result of which silicon is actively involved in surface diffusion, inhibiting the displacement of gold atoms.

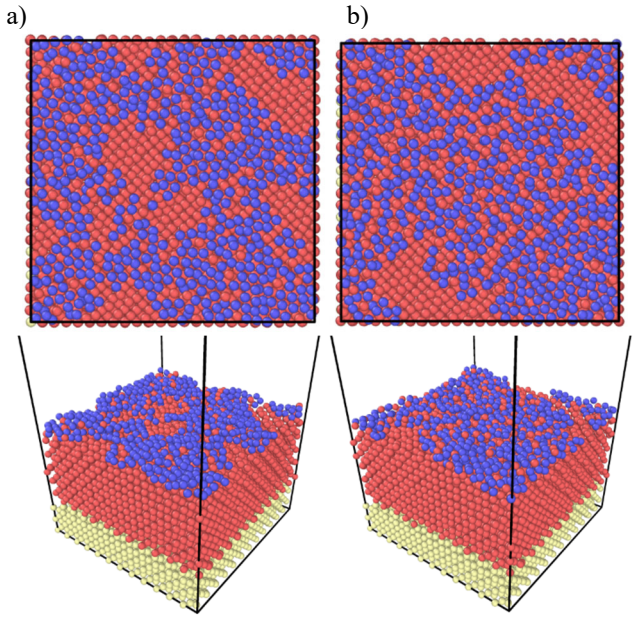

Fig. 16. Visualization of 1 ML system at 575 K (a) and 625 K (b)

4. Conclusions

Simulation of the surface diffusion of gold atoms on the silicon (111) surface indicates the preference interaction between them in a wide temperature range. As a result, a clustering of gold atoms was observed.

It is clear that the behaviour of gold atoms on the surface of silicon depends on the features of the interatomic interaction forces and the temperature of the system. In the case of the movement of one atom on the surface of silicon the main mechanism of its jumps is random walk and interstitial diffusion. During its movement, the gold atom makes several jumps and after each of them, it proceeds to oscillate at the subsequent interstitial positions. At high temperatures, the gold atom may also move down into the first or second silicon atomic planes.

Two gold atoms on the surface of silicon try to form pairs whose behaviour depends on temperature. At a temperature close to 675 K, the pair of Au atoms travels together at short distances. As the temperature increases, the pair of gold atoms has fewer preferable jump positions, because the size

of the atomic pair is larger than a single atom. In case of the temperature distortion of the silicon substrate, observed at the end of the simulation, the system of two atoms did not move far from the initial position, instead oscillating in their original position.

Analysis of the behaviour of four gold atoms on the surface of silicon identified three possible mechanisms of their motions. The first is that each individual atom performs a certain number of jumps and connected into a cluster. The second mechanism appears when only three out of four gold atoms form a cluster. The third case is observed when during large oscillations of the silicon substrate, the four atoms disconnect completely from each other and the cluster is not formed. This behaviour has been observed e.g. at temperature of 925 K.

It was shown that, for the case of an incompletely filled silicon surface with gold atoms, an increase in temperature leads to an increase in the number of displacements of the gold atoms, which commensurate with the size of the silicon atom. In this case, the activation energy of single atomic displacement decreases with increasing number of gold atoms. For the case of a completely filled silicon surface with gold the number of large jumps decreases with increasing temperature. Analysis of the temperature dependences of the average interatomic distances indicates that the temperature stability of gold clusters decreases with decreasing number of atoms in the cluster.

The research results can be used to select the modes of gold sputtering to create gold nanoislands or nanopillars on the silicon surface.

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References

[1] M.K. Bayazit, J. Yue, E. Cao, A. Gavriilidis, J. Tang, Controllable Synthesis of Gold Nanoparticles in Aqueous Solution by Microwave Assisted Flow Chemistry, ACS Sustainable Chemistry and Engineering 4/12 (2016) 6435-6442. DOI: https://doi.org/10.1021/acssuschemeng.6b01149

[2] M.A. El-Sayed, Some Interesting Properties of Metals Confined in Time and Nanometer Space of Different Shapes, Accounts of Chemical Research 34/4 (2001) 257-264. DOI: https://doi.org/10.1021/ar960016n

[3] D.E. Mustafa, T. Yang, Z. Xuan, S. Chen, H. Tu, A. Zhang, Surface Plasmon Coupling Effect of Gold Nanoparticles with Different Shape and Size on Conventional Surface Plasmon Resonance Signal, Plasmonics 5/3 (2010) 221-231. DOI: DOI: https://doi.org/10.1007/s11468-010-9141-z

[4] E. Piscopiello, L. Tapfer, M. Vittori Antisari, P. Paiano, P. Prete, N. Lovergine, Formation of epitaxial gold nanoislands on (100) silicon, Physical Review B – Condensed Matter and Materials Physics 78/3 (2008) 035305. DOI: https://doi.org/10.1103/PhysRevB.78.035305

[5] S. Eustis, M.A. El-Sayed, Why gold nanoparticles are more precious than pretty gold: Noble metal surface plasmon resonance and its enhancement of the radiative and nonradiative properties of nanocrystals of different shapes, Chemical Society Reviews 35/3 (2006) 209-217. DOI: https://doi.org/10.1039/B514191E

[6] L. Wang, G.A. Hudson, Advanced Molecular Dynamics Simulations on the Formation of Transition Metal Nanoparticles, in: L. Wang (ed.), Molecular Dynamics – Theoretical Developments and Applications in Nanotechnology and Energy, IntechOpen, Rijeka, 2012, 25-42. DOI: https://doi.org/10.5772/36344

[7] D. Bahloul-Hourlier, P Perrot, Thermodynamics of the Au-Si-O system: Application to the synthesis and growth of silicon-silicon dioxide nanowires, Journal of Phase Equilibria and Diffusion 28/2 (2007) 150-157. DOI: https://doi.org/10.1007/s11669-007-9023-z

[8] A, Gapska, M. Łapiński, P. Syty, W. Sadowski, J.E. Sienkiewicz, B. Kościelska, Au-Si plasmonic platforms: synthesis, structure and FDTD simulations, Beilstein Journal of Nanotechnology 9 (2018) 2599-2608. DOI: https://doi.org/10.3762/bjnano.9.241

[9] W. Święch, E. Bauer, M Mundschau, A low energy electron microscopy study of the system Si (111)-Au, Surface Science 253/1 (1991) 283-296. DOI: https://doi.org/10.1016/0039-6028(91)90599-N

[10] S.S. Kosolobov, A.V. Latyshev, Atomic steps on the Si(111) surface during submonolayer gold adsorption, Bulletin of the Russian Academy of Sciences: Physics 72/2 (2008) 176-180. DOI: https://doi.org/10.1007/s11954-008-2010-7

[11] B. Smoljan, D. Iljkić, M. Maretić, Computer simulation of hardness and microstructure of casted steel 100Cr6, Archives of Materials Science and Engineering 78/1 (2016) 23-28. DOI: https://doi.org/10.5604/18972764.1226312

[12] T. Linek, T. Tański, W. Borek, Numerical analysis of the cavitation effect occurring on the surface of steel constructional elements, Archives of Materials

Science and Engineering 85/1 (2017) 24-34. DOI: https://doi.org/10.5604/01.3001.0010.1555
[13] A. Śliwa, Application of the Finite Elements Method for computer simulation of properties of surface layers, Archives of Materials Science and Engineering 86/2 (2017) 56-85. DOI: https://doi.org/10.5604/01.3001.0010.4886
[14] V. Plechystyy, I Shtablavyi, S. Winczewski, K. Rybacki, S. Mudry, J. Rybicki, Structure of the interlayer between Au thin film and Si-substrate: Molecular Dynamics simulations, Materials Research Express 7/2 (2020) 026553. DOI: https://doi.org/10.1088/2053-1591/ab5e76
[15] L.J. Lewis, P. Jensen, N. Combe, J.L. Barrat, Diffusion of gold nanoclusters on graphite, Physical Review B – Condensed Matter and Materials Physics 61/23 (2000) 16084-16090. DOI: https://doi.org/10.1103/PhysRevB.61.16084
[16] P. Deltour, J.-L. Barrat, P. Jensen, Fast Diffusion of a Lennard-Jones Cluster on a Crystalline Surface, Physical Review Letters 78/24 (1997) 4597. DOI: https://doi.org/10.1103/PhysRevLett.78.4597
[17] S. Plimton, Fast Parallel Algorithms for Short- Range Molecular Dynamics, Journal of Computational Physics 117/1 (1995) 1-19. DOI: https://doi.org/10.1006/jcph.1995.1039
[18] S. Ryu, W. Cai, Molecular dynamics simulations of gold-catalyzed growth of silicon bulk crystals and nanowires, Journal of Materials Research 26/17 (2011) 2199-2206. DOI: https://doi.org/10.1557/jmr.2011.155
[19] A. Stukowski, Visualization and analysis of atomistic simulation data with OVITO-the Open Visualization Tool, Modelling and Simulation in Materials Science and Engineering 18/1 (2010) 015012. DOI: https://doi.org/10.1088/0965-0393/18/1/015012
[20] P.E. Batson, Motion of Gold Atoms on Carbon in the Aberration-Corrected STEM, Microscopy and Microanalysis 14/1 (2008) 89-97. DOI: https://doi.org/10.1017/S1431927608080197