01

Molecular dynamics study of reversible relaxation of compressive mechanical stress in polycrystalline metal films after the interruption of their deposition

© *A.S. Babushkin, A.N. Kupriyanov*

Valiev Institute of Physics and Technology of RAS, Yaroslavl Branch,
150007 Yaroslavl, Russia
e-mail: artem.yf-ftian@mail.ru

Received April 12, 2023
Revised August 23, 2023
Accepted August 24, 2023

The results of MD simulation of polycrystalline metal films deposition are presented. Using Cr and Cu as an example, the influence of the deposited particle energy, the deposition rate, as well as the film material and temperature on the change in stress upon interruption and resuming deposition is studied. The simulation results showed that the reversible relaxation of compressive stress in polycrystalline films upon interruption of deposition is associated with the lateral displacement of atoms trapped in grain boundaries from the surface during deposition. This process of redistribution of atoms in grain boundaries leads to their more compact arrangement and proceeds in the same way in all layers of the film, both after and during deposition. The higher the mobility of atoms on the surface due to the type of material, temperature or energy of the deposited particles and the higher the rate of deposition, the greater the change in stress when it stops. No escape of atoms from grain boundaries back to the film surface was observed when deposition was interrupted.

Keywords: residual mechanical stress, polycrystalline film growth, chromium, copper, molecular dynamics.

DOI: 10.61011/TP.2023.10.57442.92-23

Introduction

Thin polycrystalline films of metals are widely used in micro- and nanoelectromechanical systems [1,2], optics [3] and storage devices [4]. Residual mechanical stress occurring during deposition limit the possibility of their use, as they can lead to cracking and peeling [5,6], swelling of the film [6,7], as well as deformation of structural elements [8]. On the other hand, controlled deformation caused by residual stress can be used for self-assembly of three-dimensional MEMS devices [9–12].

It is necessary to understand the mechanisms of their formation during the deposition of films to predict and control stress.

Most metal films grow according to the Volmer-Weber mechanism [13], during which three stages of stress formation are defined. Separate islands with compressive stress are formed on the substrate at the initial stage. These stress are associated with the Laplace pressure [14], as well as the influence of surface defects [15]. At the second stage, the islands begin to touch and form an grain boundary, which leads to a decrease of surface energy [16–18]. As a result, tensile stress occur in the film. The film continues to accumulate tensile stress at the third stage, with low mobility of adatoms. The tensile stress will decrease and a transition to compressive stress will gradually occur if the mobility of adatoms is high [19,20]. The amount of mobility of adatoms depends on both the material and the deposition conditions, for example, the temperature of the substrate and the energy of the deposited atoms. When deposition stops, some of these compressive stress relax, and if deposition is resumed, the stress return to the previous value and develop as if there was no break [20,21]. The mechanism of the occurrence of compressive stress at this stage and their partial relaxation when deposition stops is still being discussed [22–24]. The reasons are the penetration of adatoms into the grain boundary and their exit back to the surface [17], the ingress of adatoms between coalescing atomic steps and their return exit [25], inheritance of compressive stress from the first stage of film growth and recrystallization, which leads to a change in density grain boundaries [26].

The most generalized kinetic model describing the formation of stress during the deposition of polycrystalline films is presented in [27,28]. This model directly relates the magnitude of stress to the deposition parameters and microstructure and, as a result, well explains the stress dependences observed in experiments on the deposition rate, temperature and film material. The authors attribute the occurrence of tensile stress to the formation of a grain boundary and a decrease of surface energy, and the occurrence of compressive stress is explained by the penetration of adatoms into the grain boundaries. They believe that the latter is caused by an increase of the chemical potential on the surface ($\delta\mu_s$) of grains because during deposition it comes to a non-equilibrium state. The resulting difference of chemical potentials on the surface and in the grain boundary $\Delta\mu$ becomes the driving force

for adatoms. It is equal to $\delta\mu_s + \sigma_i\Omega$, where σ_i — stress in the near-surface atomic layer, Ω — volume per atom. The plus sign is due to the fact that compressive stress are considered negative. During deposition, $\Delta\mu$ is positive, resulting in the movement of adatoms from the surface into the grain boundary and the formation of compressive stress. The formation of a new section of the grain boundary results in the occurrence of tensile stress in the new atomic layer, after which the introduction of adatoms into it leads to a gradual decrease of tensile stress and transition to compressive stress. This sequence of processes is repeated in each new atomic layer i, producing stress in it σ_i:

$$\sigma_i = \sigma_C + (\sigma_T - \sigma_C)\exp\left(-\frac{\Delta t_i}{\tau}\right), \qquad (1)$$

where σ_T — tensile stress occurring during the formation of a new section of the grain boundary in the i layer, σ_C — maximum compressive stress that may occur in it as a result of the introduction of adatoms into the grain boundary, Δt_i — layer formation time, and τ — kinetic parameter depending on grain size L, lattice parameter a and effective diffusion coefficient D:

$$\tau = \frac{La}{\beta D}. \qquad (2)$$

The constant β — is defined as follows:

$$\beta = \frac{4C_s M_f \Omega}{kT}, \qquad (3)$$

where Ω — volume per atom, M_f — biaxial module, C_s — ratio of the number of mobile atoms to the number of seats on the terrace adjacent to the grain boundary, k — Boltzmann constant, T — temperature.

As a result, the average stress in a film with a thickness of h having N filled atomic layers are equal to

$$\langle\sigma\rangle = \frac{a}{h}\sum_i\left[\sigma_C + (\sigma_T - \sigma_C)\exp\left(-\frac{\Delta t_i}{\tau}\right)\right]. \qquad (4)$$

The authors of the kinetic model believe that the chemical potential on the surface returns to the equilibrium state, the additive $\delta\mu_s$ disappears, and in the presence of compressive stress $\Delta\mu$ becomes negative when the deposition stops and as a result part of the atoms returns back to the surface [24].

A capability to observe the behavior of individual atoms during the deposition of the film and after the deposition stops is needed to study which processes lead to the formation and relaxation of stress in the film. Unfortunately, the capabilities of existing experimental methods for studying films *in-situ* are very limited. However, modern methods of computer modeling, in particular the method of molecular dynamics (MD), open up more and more opportunities for the study of processes occurring at the atomic level. Modeling is performed by solving equations of motion to obtain the positions of all atoms in the model as functions of time. The forces acting on each atom are determined by the interatomic interaction potential set by the user. Many papers have covered modeling of the deposition of metal films by the method of molecular dynamics, but only a small part of them consider polycrystalline films. The penetration of adatoms into the grain boundary during the deposition of Ni films, in which compressive stress were formed as a result, was demonstrated in [29,30]. The results of an extensive study of the dependence of the stress formation process during the growth of Fe and W polycrystalline films on such parameters as the shape, size, orientation of the initial islands and the energy of the deposited atoms are provided in [31]. The stress changes during deposition in their paper are consistent with the kinetic model. However, the exit of atoms from the grain boundary back to the surface was not detected during the simulation of the process of relaxation of compressive stress with the stopped deposition, but it was noticed that the width of the grain boundary in the near-surface region decreases after deposition ceases. We studied the dependence of surface roughness and mechanical stress on the energy of deposited atoms and the deposition rate in our paper covering the modeling of the deposition of polycrystalline films Cr [32]. The higher the energy of the atoms and the lower the deposition rate, the more atoms were able to descend the atomic steps, complete them and penetrate into the grain boundary. As a result, films deposited with higher energies had a smoother surface and higher compressive stress. A decrease of the deposition rate also led to an increase of compressive stress, but the surface roughness practically did not change. These results are quite consistent with the kinetic model. However, the study of the deposition stop demonstrated that the partial relaxation of compressive stress is not associated with the release of atoms back to the surface, but with their redistribution in the grain boundary in the lateral direction. Thus, despite a good consistency of mechanisms of stress formation presented in the kinetic model during the deposition of films with the results of experiments and MD simulations, its description of the relaxation of compressive stress after the deposition stops is not consistent with the results of MD simulations.

The purpose of this work is to study by the method of molecular dynamics of stress changes during stopping and resuming deposition of polycrystalline films to find out what exactly causes the effect of reversible relaxation of compressive stress, to study the impact of the energy of the deposited particles, the deposition rate, as well as the temperature and the film material.

1. Model description

The simulation was conducted using a freeware package for solving problems of molecular dynamics LAMMPS [33]. Data were visualized using open source software for the analysis of particle-based models OVITO [34]. The

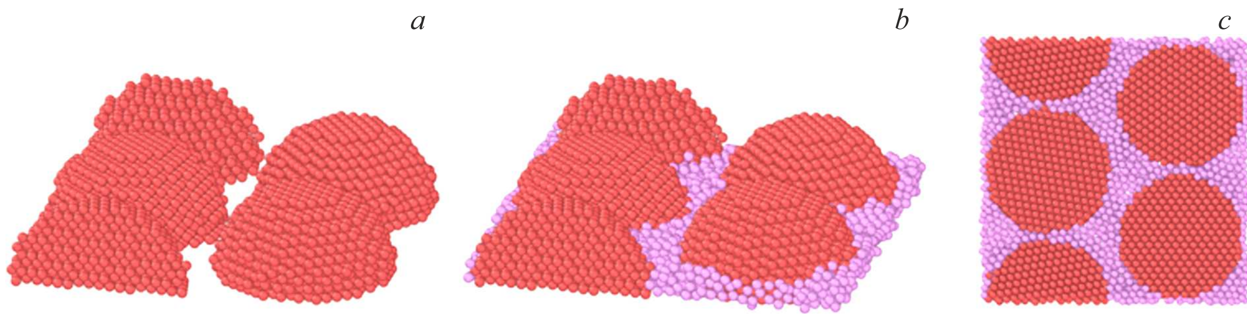

Figure 1. Image of the model before deposition: hemispherical islands before (a) and after (b) formation of the initial thin layer of the grain boundary, as well as a bottom view (c).

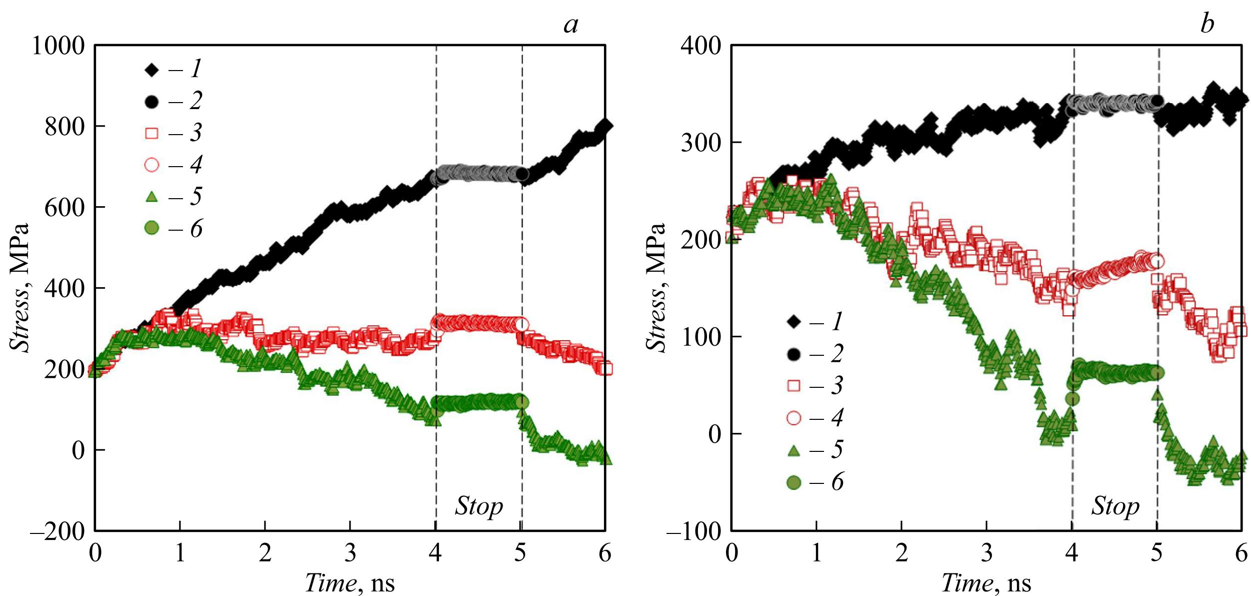

Figure 2. Change of mechanical stress during deposition of films Cr (a) and Cu (b) with incident particle energies 3 (*1*), 10 (*3*) and 15 eV (*5*) at 300 K, as well as stopping (*2, 4, 6*) and resuming (*1, 3, 5*) deposition.

submerged atom model [35] was used to calculate the interaction between Cu atoms, and a modified submerged atom mode was used to calculate the interaction between between Cr atoms [36]. The simulation step was equal to 1 fs. Hemispherical islands with orientation (110) were formed to simulate a polycrystalline Cr film at the initial stage of growth, (Cr films deposited by the magnetron method in our experimental studies had this texture [37,38]) and a radius of 2 nm (Fig. 1, a), the space between them was filled with a thin layer of amorphous phase (Fig. 1, b). Cu films were produced in a similar manner, but with orientation (111), since such a texture is most characteristic of metal films with a FCC lattice [39]. This approach to modeling the deposition of polycrystalline films is described in more detail in [31]. Three of the four crystallites were rotated relative to the axis of symmetry of the hemisphere at angles -45°, 45° and 90° (Fig. 1, c), as a result, during deposition, the grains did not coalesce into a single single-crystal, but a disordered grain boundary was formed. The lower layer of atoms in the hemispheres was fixed. The space between the grains at the height of four atomic layers was filled with atoms randomly. The density of filling of these four layers determined the value of the initial stress in the film [31]. The lower layer of this group of atoms was also fixed, but only along the Z axis, as a result of which they were rearranged after the free energy minimization procedure forming the beginning of the grain boundary. Periodic boundary conditions were set on the side faces of the modeling area. Before the deposition, a temperature equal to 300 K was set in the entire model and a relaxation procedure was performed. 300 K thermostat was set above a fixed layer during the deposition in three atomic layers.

The atoms were thrown every 500 fs at a height of 8 nm from the sample. The horizontal coordinates of the point of occurrence of the atom were determined randomly. The initial velocity corresponding to the required kinetic energy

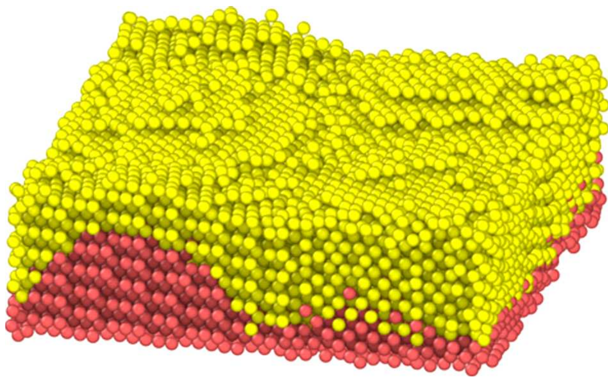

Figure 3. Image of a Cr film model after deposition for 4 ns with an energy of 15 eV and a deposition period of 500 fs.

and directed vertically downward was set for the deposited atoms.

The components of the stress tensor were determined using kinetic energy and virial [40]:

$$\sigma_{ij} = -\left(\frac{\sum_{k}^{N} m_k v_{ki} v_{kj}}{V} + \frac{\sum_{k}^{N'} r_{ki} f_{kj}}{V} \right), \tag{5}$$

where i and j take the values x, y and z; m — atom mass, V — the volume occupied by N atoms, v_{ki} and v_{kj} — the velocity components of kth atom, r_{ki} and f_{kj} — components of the radius vector and the force acting on the kth atom, respectively. Since the film is free in the vertical direction, the stress component σ_{zz} is zero. The horizontal stress components in isotropic films are equal, but at each moment, due to fluctuations in the model, they could differ slightly, so averaging was carried out, and the final stress value was determined as $(\sigma_{xx} + \sigma_{yy})/2$.

2. Findings and discussion

Figure 2 shows the change in mechanical stress during the deposition of films Cr (a) and Cu (b) with incident particle energies 3, 10 and 15 eV during 4 ns, as well as during the deposition stop during 1 ns and renewals for 1 ns. As you can see, there are some oscillations on all charts during deposition. At first glance, it may seem that this is just noise, but it is not. Each value on the graph is the result of averaging 100 measurements performed at each of the 100 steps. These oscillations are quite consistent with the kinetic model. When a new atomic layer arises and a new section of the grain boundary appears, it immediately introduces an addition of tensile stress. Further, the tensile stress in this layer gradually decrease and can turn into compressive ones. As a result, we see oscillations on the mean stress plot , since the model is small (Fig. 3) (for 4 ns, 8 more are added to the original 4 completed atomic layers), and the contribution of each new layer to the total stress is quite noticeable.

In the same deposition conditions, the stress change plots in Cu films are shifted towards compressive stress compared to stress change plots for Cr. This is due to the fact that Cu atoms have higher mobility, and therefore, during deposition, more atoms are able to penetrate from the surface into the grain boundary. Similarly, the amount of energy of the deposited particles affects. At the energy of the incident particles 3 eV, the atoms on the surface have low mobility, so only a small part of them is able to reach the grain edge and penetrate into the grain boundary, and as a result, tensile stress mainly develop in the films. At higher

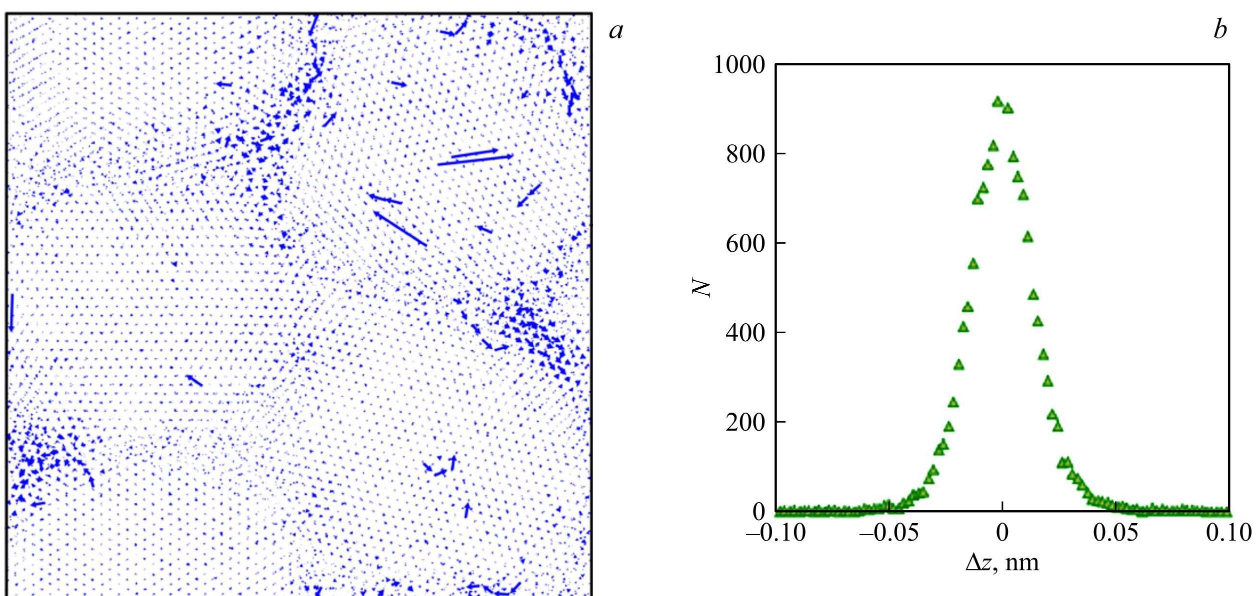

Figure 4. The displacement vectors of the atoms Cu during 1 ns after the film deposition with the energy of incident particles 15 eV during 4 ns (a), the distribution of the vertical components of these vectors (b).

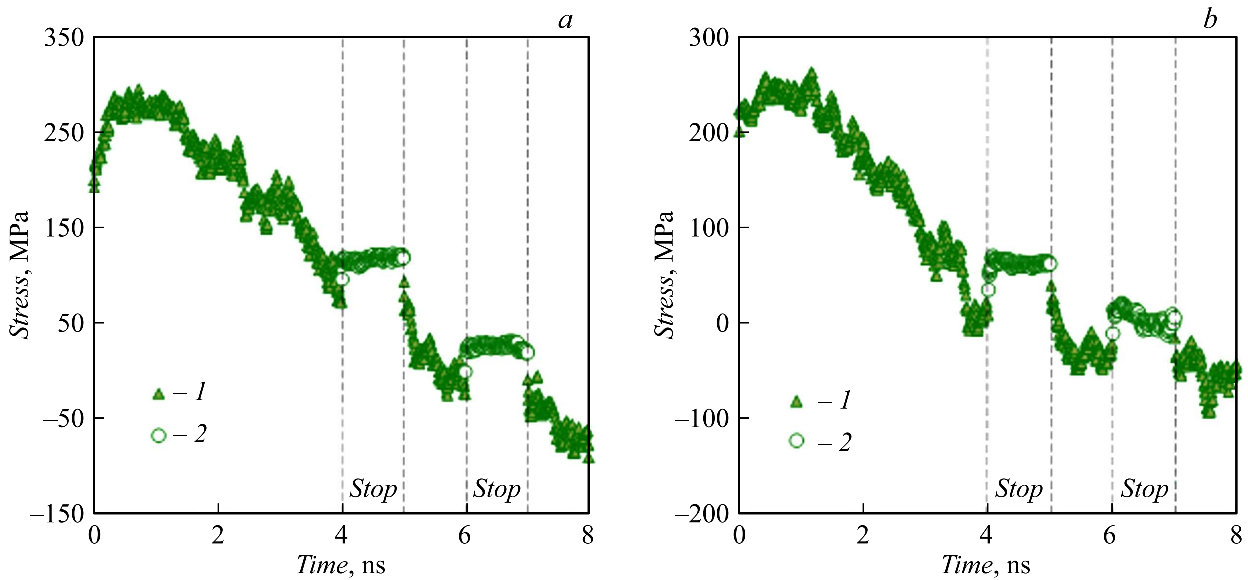

Figure 5. The change in mechanical stress in the films Cr (a) and Cu (b) during deposition with an energy of 15 eV (1) and two consecutive deposition stops (2).

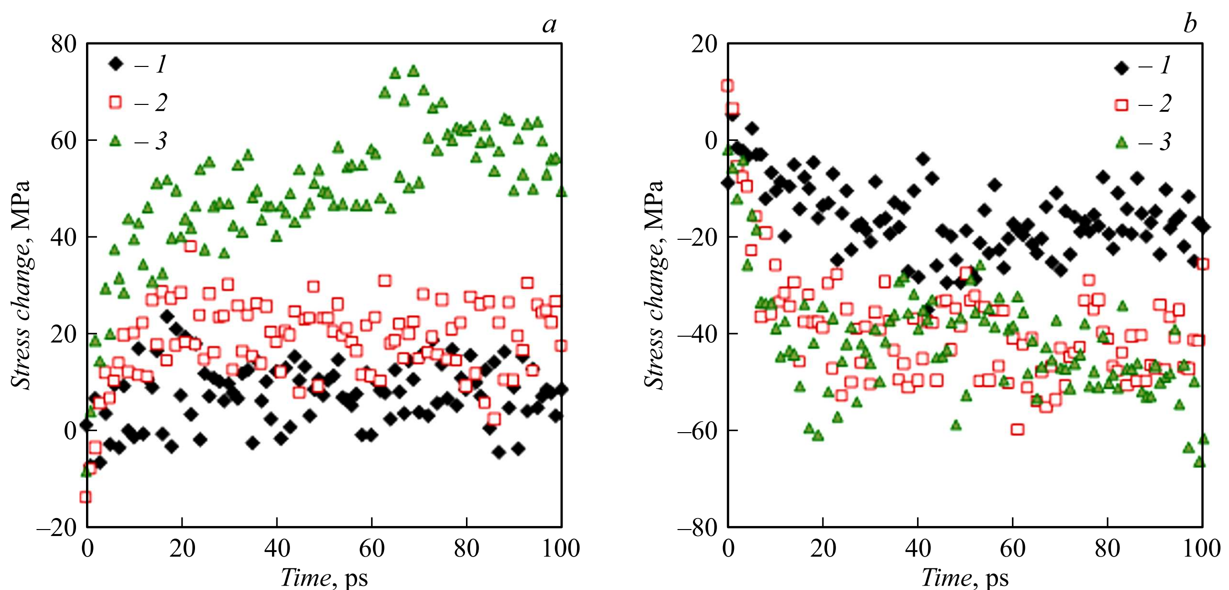

Figure 6. Change in mechanical stress in the first 100 ps after stopping (a) and resuming (b) deposition of Cu films with incident particle energies of 3 (1), 10 (2) and 15 eV (3) at 300 K.

energies, the atoms on the surface have higher mobility, which results in a gradual transition from tensile stress to compressive stress during deposition.

The same is reflected and on the magnitude of the stress change when the deposition stops. Earlier, when modeling the deposition of Cr films, we showed that this change is due to the redistribution of atoms inside the grain boundary [41]. The higher the mobility of atoms, the more they penetrate into the grain boundary and the greater the effect of restructuring. Therefore, the change in stress after the deposition stops in Cu films is greater than in Cr films, and it also increases with increasing energy of the deposited atoms. At the same time, the no release of atoms to the surface was observed, as in the previous work. Figure 4 shows the displacement vectors of Cu atoms after the deposition stops (top view) with the energy of the incident particles 15 eV by 1 ns (a), as well as a graph of the distribution of their vertical components (b). It can be seen that the redistribution of atoms occurs in the grain boundary. The displacements are so small in the area of grains (except for a few atoms on the surface) that the arrows have degenerated into dots. The plot of the distribution of the

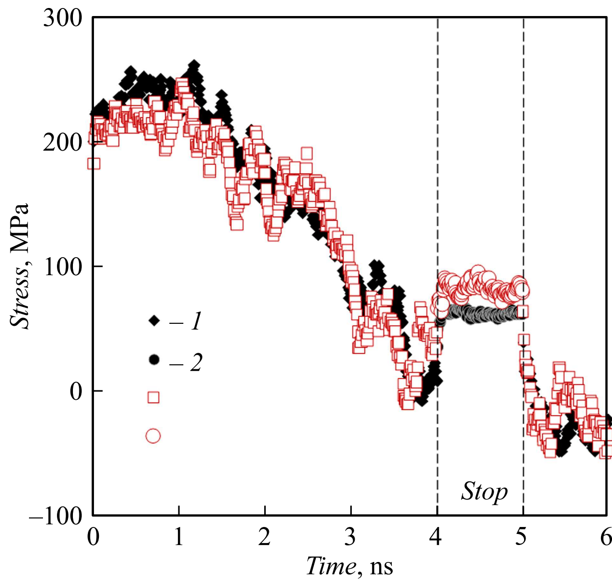

Figure 7. Change of mechanical stress during deposition of films Cu with the energy of incident particles 15 eV at 300 (*1*) and 500 K (*3*), as well as stopping (*2, 4*) and resuming (*1, 3*) deposition.

vertical components of the displacement vectors shows that there is no directional movement of atoms vertically.

Figure 5 shows the result of two consecutive stops of deposition of films Cr (*a*) and Cu (*b*). The values of the voltage changes during the first and second stops are almost the same. This suggests that the process of rearrangement of atoms does not depend on the stress in the underlying layers, since during the first and second deposition stops, the average stress in the films differed in both magnitude and sign.

Fig. 6 shows plots of stress changes in Cu films deposited with incident particle energies 3, 10 and 15 eV in the first 100 ps after the deposition was stopped for 4 ns (*a*), and in the first 100 ps after its resumption (*b*). These plots are given for a more detailed consideration of the results of stopping and resuming deposition, presented in Fig. 2, *b*. Each value in these plots is the result of averaging 1000 measurements taken at each step. The higher the energy of the deposited atoms, the greater the change in stress when the deposition stops and resumes. As mentioned earlier, this is probably due to the fact that with greater mobility on the surface, more adatoms penetrate into the grain boundary. The more of them there are in a limited space, the more they tend to redistribute more compactly. Also in Fig. 5, a it can be seen that the relaxation time for all energies is approximately the same. Apparently, this is due to the fact that on the way from the surface to the grain boundary, adatoms lose their energy and already in the grain boundary their mobility does not differ from that of the surrounding atoms.

The rapid return of the initial stress state after the resumption of deposition is probably due to a temporary increase of the flow of adatoms from the surface to the grain boundary, caused by the fact that the difference in chemical potentials between them increased during the shutdown due to partial relaxation of compressive stress.

Fig. 7 shows the change in mechanical stress during deposition of Cu films with the energy of incident particles 15 eV at temperatures of 300 and 500 K, as well as during stopping and resuming deposition. Stress changes after stopping and resuming deposition are shown in more detail in Fig. 8. In general, the plots of stress changes during deposition are quite close. At first glance, it may seem that the relaxation during a stop at 500 K is slightly greater, but

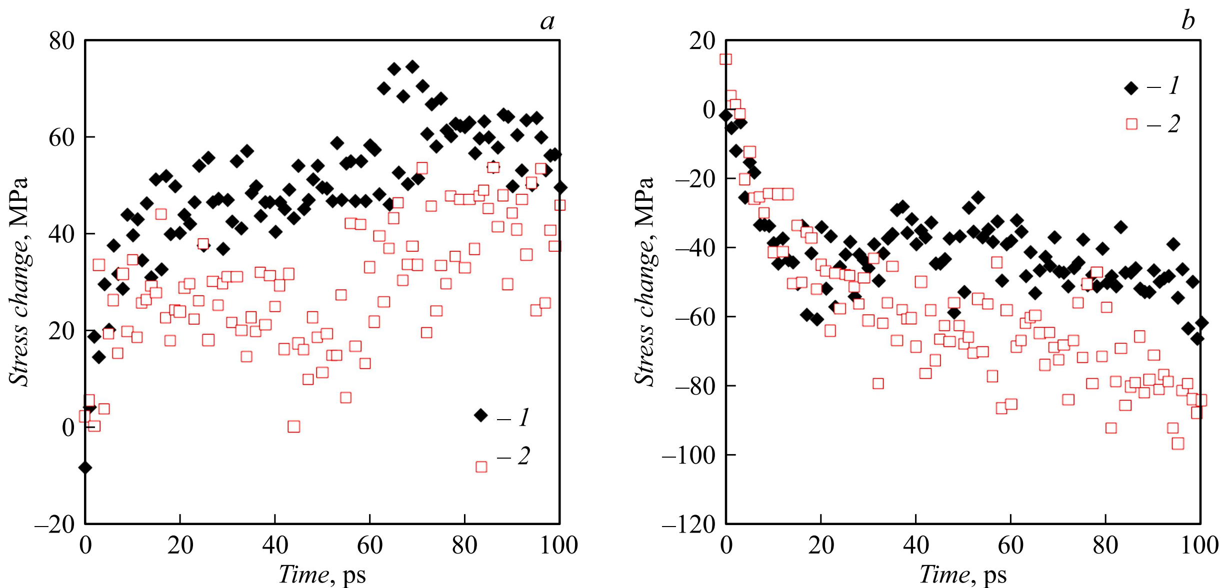

Figure 8. Change in mechanical stress in the first 100 ps after stopping (*a*) and resuming (*b*) deposition of films Cu with the energy of incident particles 15 eV at 300 (*1*) and 500 K (*2*).

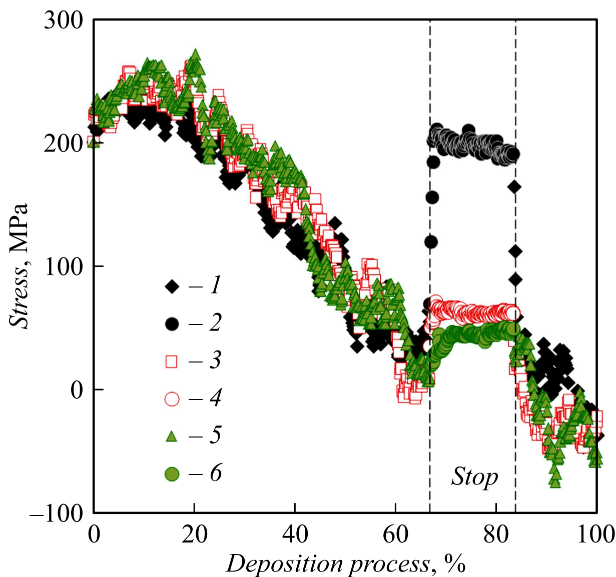

Figure 9. Change in mechanical stress during deposition of Cu films with the energy of incident particles 15 eV at 300 K with periods between atom throws 125 (*1*), 500 (*3*) and 2000 fs (*5*), as well as stopping (*2, 4, 6*) and resuming (*1, 3, 5*) deposition.

it is the change in stress that is actually less than at 300 K (Fig. 8, *a*).

This may seem contradictory, because with greater mobility, more atoms should penetrate into the grain boundary, which will subsequently result in a large restructuring and an effect on stress. But the fact is that the redistribution of atoms in the grain boundary occurs not only after stopping, but also during deposition. Atoms penetrate into the grain boundary, there is less and less free space and they begin to rebuild. This process occurs in all layers during deposition and what we see after it stops — is only a residual phenomenon. At the same time, the relaxation rate depends on the mobility of atoms in the grain boundary, and therefore on the temperature of the thermostat. Since at 500 K the relaxation process proceeds faster, by the time the deposition stops, the greater part of it has already been completed than at 300 K. Therefore, the stress changes after the deposition stops at 500 K are less than at 300K.

Fig. 9 shows the result of deposition of films of Cu with the energy of incident particles 15 eV at 300 K with periods between throws of atoms 125, 500 and 2000 fs, as well as its stops and resumes. Percentages are used for the abscissa axis due to the difference in time scales. Stress changes after stopping and resuming deposition in the first 10% of the time are shown in more detail in Fig. 10. As you can see, the faster the film was deposited, the more the stress changed after the deposition stopped. As mentioned earlier, the process of redistribution of atoms in the grain boundary proceeds, including during the deposition itself. Therefore, the faster the film is deposited, the smaller the fraction of relaxation has time to occur during deposition and the greater part of it continues to flow after stopping. As a result, the higher the deposition rate, the greater the stress change after it stops.

Conclusion

The results of MD modeling show that the reversible relaxation of compressive stress in polycrystalline films when deposition stops is associated with the redistribution of atoms inside the grain boundaries. The atoms move laterally, resulting in a more compact arrangement. No release of atoms back to the surface of the film was observed

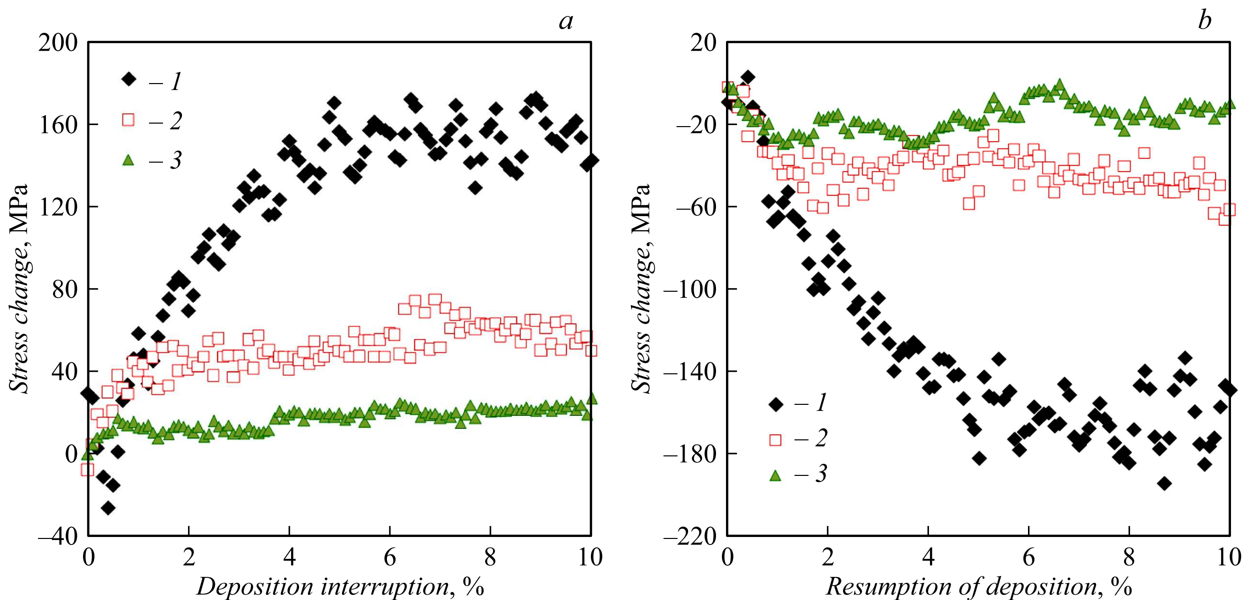

Figure 10. Change in mechanical stress in the first 10% of the time after stopping (*a*) and resuming (*b*) deposition of films Cu with the energy of incident particles 15 eV at 300 K with periods between atom throws 125 (*1*), 500 (*2*) and 2000 fs (*3*).

when the deposition was stopped. The atom rearrangement process does not depend on the stress in the underlying layers. The higher the mobility of atoms on the surface and the deposition rate, the greater the stress change when it stops.

Funding

The work has been performed under the state assignment to the Valiev Institute of Physics and Technology of RAS of the Ministry of Education and Science of the Russian Federation on the topic FFNN-2022-0017.

Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] V.K. Varadan, K.J. Vinoy, K.A. Jose. *RF MEMS and Their Applications* (John Wiley & Sons, Ltd, Chichester, UK, 2002), DOI: 10.1002/0470856602

[2] J. Laconte, D. Flandre, J.P. Raskin. *Micromachined thin-film Sensors for SOI-CMOS Co-integration* (Springer Science & Business Media, 2006), DOI: 10.1007/0-387-28843-0

[3] J.-H. Cho, M.D. Keung, N. Verellen, L. Lagae, V.V. Moshchalkov, P. Van Dorpe, D.H. Gracias. Small, **7** (14), 1943 (2011). DOI: 10.1002/smll.201100568

[4] A.V. Fadeev, K.V. Rudenko. Russ. Microelectron., **50**, 311 (2021). DOI: 10.1134/S1063739721050024

[5] Z.C. Xia, J.W. Hutchinson. J. Mech. Phys. Solids, **48** (6-7), 1107 (2000). DOI: 10.1016/S0022-5096(99)00081-2

[6] K.A. Valiev, R.V. Goldstein, Y.V. Zhitnikov, T.M. Makhviladze, M.E. Sarychev. Russ. Microelectron., **38**, 364 (2009). DOI: 10.1134/S106373970906002X

[7] M.W. Moon, J.W. Chung, K.R. Lee, K.H. Oh, R. Wang, A.G. Evans. Acta Mater., **50** (5), 1219 (2002). DOI: 10.1016/S1359-6454(01)00423-2

[8] S. Dutta, M. Imran, R. Pal, K.K. Jain, R. Chatterjee. Microsyst. Technol., **17**, 1739 (2011). DOI: 10.1007/s00542-011-1360-5

[9] D. Karnaushenko, T. Kang, V.K. Bandari, F. Zhu, O.G. Schmidt. Adv. Mater., **32** (15), 1902994 (2020). DOI: 10.1002/adma.201902994

[10] D.D. Karnaushenko, D. Karnaushenko, D. Makarov, O.G. Schmidt. NPG Asia Mater., **7** (6), e188 (2015). DOI: 10.1038/am.2015.53

[11] D. Singh, A.T. Kutbee, M.T. Ghoneim, A.M. Hussain, M.M. Hussain. Adv. Mater. Technol., **3** (1), 1700192 (2018). DOI: 10.1002/admt.201700192

[12] D.-H. Weon, J.-H. Jeon, S. Mohammadi. J. Vac. Sci. Technol. B Microelectron. Nanom. Struct, **25** (1), 264 (2007). DOI: 10.1116/1.2433984

[13] L.B. Freund, S. Suresh. *Thin film Materials: Stress, Defect Formation and Surface Evolution* (Cambridge University Press, 2004)

[14] R. Abermann, R. Kramer, J. Mäser. Thin Solid Films, **52** (2), 215 (1978). DOI: 10.1016/0040-6090(78)90140-2

[15] C. Friesen, C.V. Thompson. Phys. Rev. Lett., **89** (12), 126103 (2002). DOI: 10.1103/PhysRevLett.89.126103

[16] R.W. Hoffman. Thin Solid Films, **34** (2), 185 (1976). DOI:10.1016/0040-6090(76)90453-3

[17] W.D. Nix, B.M. Clemens. J. Mater. Res., **14** (8), 3467 (1999). DOI: 10.1557/JMR.1999.0468

[18] L.B. Freund, E. Chason. J. Appl. Phys., **89** (9), 4866 (2001). DOI: 10.1063/1.1359437

[19] G. Abadias, E. Chason, J. Keckes, M. Sebastiani, G.B. Thompson, E. Barthelf, G.L. Doll, C.E. Murray, C.H. Stoessel, L. Martinu. J. Vacuum Sci. Technol. A: Vacuum, Surfaces, and Films, **36** (2), 020801 (2018). DOI: 10.1116/1.5011790

[20] C. Friesen, S.C. Seel, C.V. Thompson. J. Appl. Phys., **95** (3), 1011 (2004). DOI: 10.1063/1.1637728

[21] J.W. Shin, E. Chason. Phys. Rev. Lett., **103** (5), 056102 (2009). DOI: 10.1103/PhysRevLett.103.056102

[22] A.R. Shugurov, A.V. Panin. Tech. Phys., **65**, 1881 (2020). DOI: 10.1134/S1063784220120257

[23] A. Jamnig, N. Pliatsikas, K. Sarakinos, G. Abadias. J. Appl. Phys., **127** (4), 045302 (2020). DOI: 10.1063/1.5130148

[24] P. Jagtap, E. Chason. Acta Mater., **193**, 202 (2020). DOI: 10.1016/j.actamat.2020.04.013

[25] A.L. Shull, F. Spaepen, J. Appl. Phys., **80** (11), 6243 (1996). DOI: 10.1063/1.363701

[26] R. Koch, D. Hu, A.K. Das. Phys. Rev. Lett., **94** (14), 146101 (2005). DOI: 10.1103/PhysRevLett.94.146101

[27] E. Chason. Thin Solid Films, **526**, 1 (2012). DOI: 10.1016/j.tsf.2012.11.001

[28] E. Chason, P.R. Guduru. J. Appl. Phys., **119** (14), 191101 (2016). DOI: 10.1063/1.4949263

[29] C.W. Pao, S.M. Foiles, E.B. Webb, D.J. Srolovitz, J.A. Floro. Phys. Rev. Lett., **99** (3), 036102 (2007). DOI: 10.1103/PhysRevLett.99.036102

[30] C.W. Pao, S.M. Foiles, E.B. Webb, D.J. Srolovitz, J.A. Floro. Phys. Rev. B - Condens. Matter. Mater. Phys., **79** (22), 224113 (2009). DOI: 10.1103/PhysRevB.79.224113

[31] X. Zhou, X. Yu, D. Jacobson, G.B. Thompson. Appl. Surf. Sci., **469**, 537 (2019). DOI: 10.1016/j.apsusc.2018.09.253

[32] A.S. Babushkin, A.N. Kupriyanov. J. Surf. Investig., **16** (6), 960 (2022). DOI: 10.1134/S1027451022060052

[33] S. Plimpton. J. Comput. Phys., **117** (1), 1 (1995). DOI: 10.1006/jcph.1995.1039

[34] A. Stukowski. Modelling and Simulation in Mater. Sci. Eng., **18** (1), 015012 (2009). DOI: 10.1088/0965-0393/18/1/015012

[35] S.M. Foiles, M.I. Baskes, M.S. Daw. Phys. Rev. B., **33** (12), 7983 (1986). DOI: 10.1103/PhysRevB.33.7983

[36] W.M. Choi, Y. Kim, D. Seol, B.J. Lee. Comput. Mater. Sci., **130**, 121 (2017). DOI: 10.1016/j.commatsci.2017.01.002

[37] A.S. Babushkin, I.V. Uvarov, I.I. Amirov. Tech. Phys., **63**, 1800 (2018). DOI: 10.1134/S1063784218120228

[38] A.S. Babushkin, R.V. Selyukov. Trudy FTIAN. Vol. 28: *Kvantovye komp'yutery, mikro- i nanoelektronika: fizika, tekhnologiya, diagnostika i modelirovanie*, ed. by T.M. Makhviladze (Nauka, M., 2019), p.112 (in Russian).

[39] W. Gruber, C. Baehtz, M. Horisberger, I. Ratschinski, H. Schmidt. Appl. Surf. Sci., **368**, 341 (2016). DOI: 10.1016/j.apsusc.2016.02.015

[40] J.F. Ziegler, J.P. Biersack. *The Stopping and Range of Ions in Matter*. In: Bromley, D.A. (eds) (*Treatise on Heavy-Ion Science*. Springer, Boston, MA. 1985), DOI: 10.1007/978-1-4615-8103-1_3

Translated by Ego Translating