MOLECULAR DYNAMICS STUDY OF REVERSIBLE RELAXATION OF COMPRESSIVE MECHANICAL STRESS IN POLYCRYSTALLINE METAL FILMS AFTER THE INTERRUPTION OF THEIR DEPOSITION

A.S. Babushkin[1,2], *A.N. Kupriyanov*[2]

1. Valiev institute of physics and technology of Russian Academy of Sciences, Moscow, Russia, *artemftian@yandex.ru*

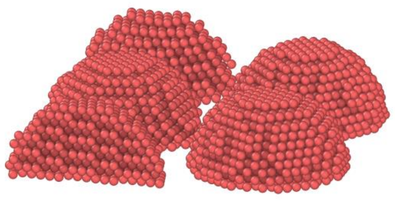
2. Valiev institute of physics and technology of Russian Academy of Sciences, Yaroslavl Branch, Yaroslavl, Russia

Abstract

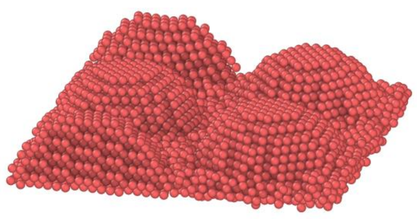
The results of MD simulation of polycrystalline metal films deposition are presented. Using Cr and Cu as an example, the influence of the deposited particle energy, the deposition rate, as well as the film material and temperature on the change in stress upon interruption and resuming deposition is studied. 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.

Model

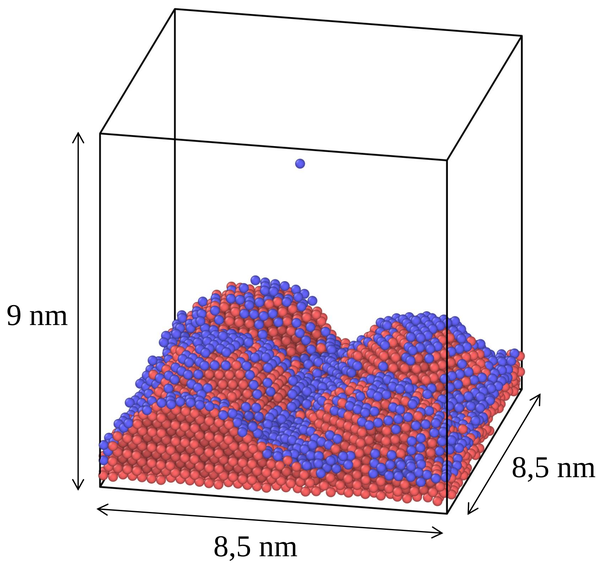
MD simulation software – LAMMPS [1]; visualization – OVITO [2].
Potentials : Cr – MEAM, Cu – EAM. The simulation step is 1 fs.



• 1. Formation of hemispherical islands.

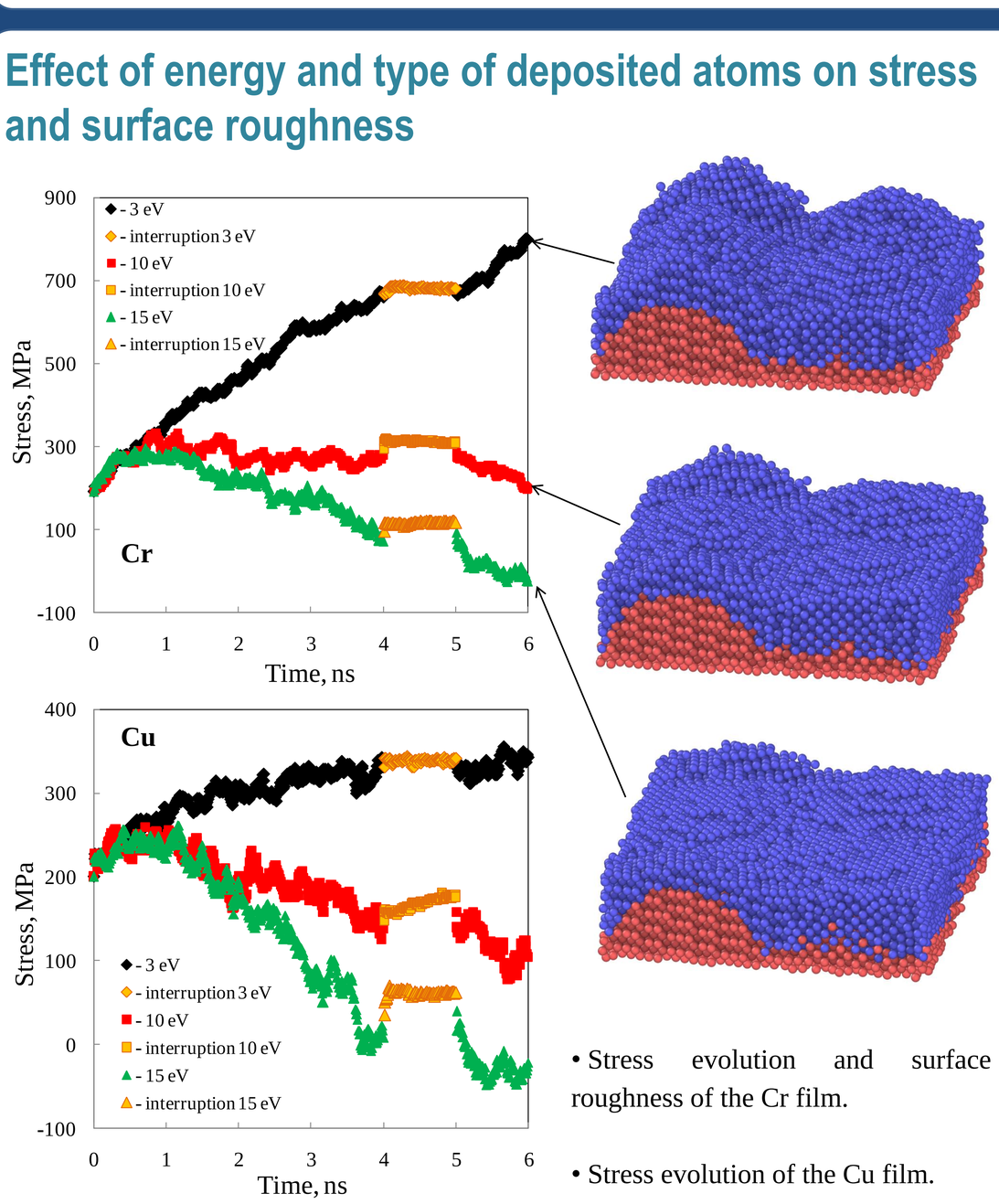


• 2. Filling of 4 atomic layers between hemispheres with disordered atoms. Enabling periodic boundary conditions on side faces. Fixation of the lower atomic layer and relaxation of the model at 300 K.



• 3. Thermostat activation in 3 lower atomic layers above the fixed layer. Generation of atoms on the upper face of the simulation area at a random point. Deposition of atoms every 500 steps.

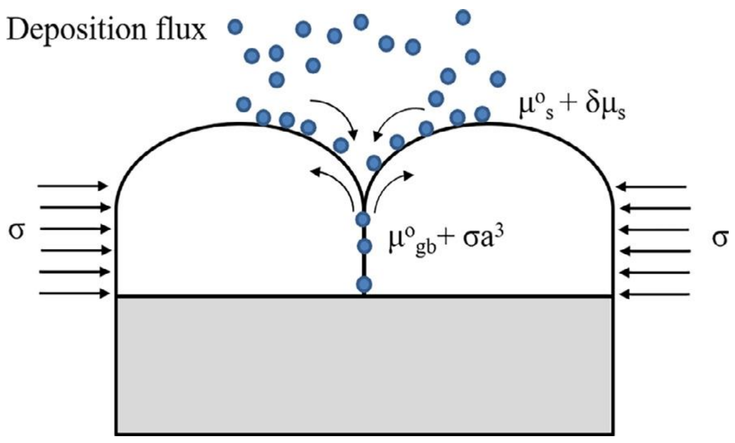
Effect of energy and type of deposited atoms on stress and surface roughness



• Stress evolution and surface roughness of the Cr film.

• Stress evolution of the Cu film.

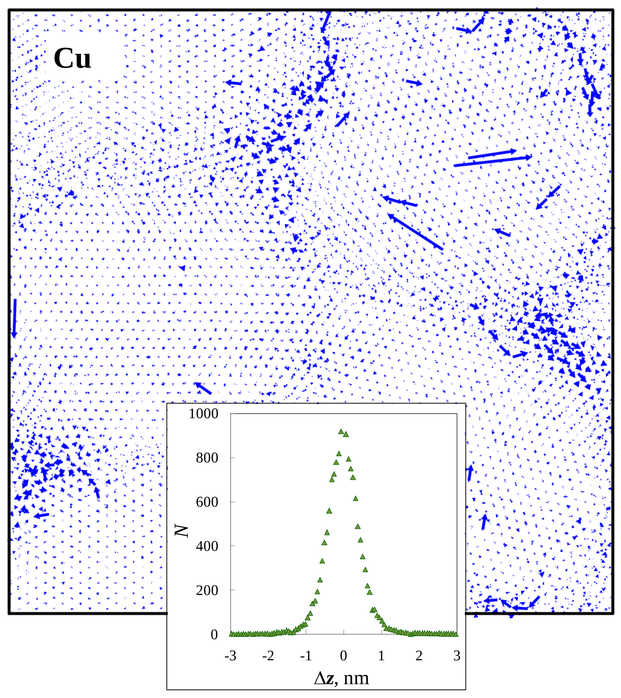
Mechanism of stress relaxation during deposition interruption



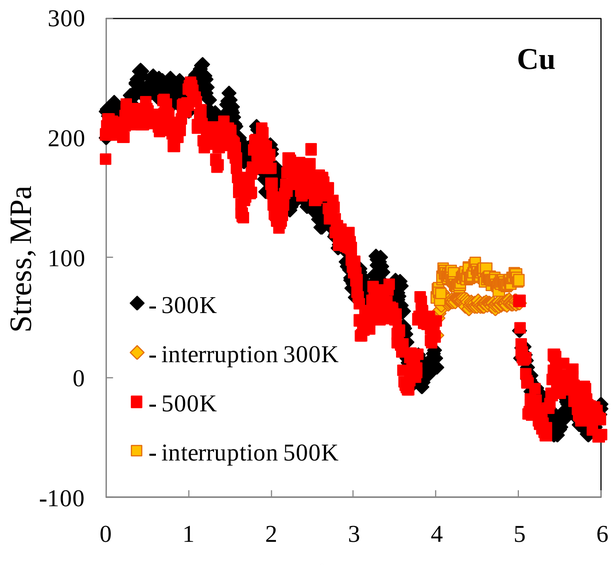
The mechanism most generally accepted in the literature is presented in [3]. During polycrystalline film deposition compressive stress are generated as a result of the penetration of adatoms from the surface into the grain boundary (GB). Its relaxation is caused by the partial release of atoms from the GB back to the surface.

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 GB. No escape of atoms from GB back to the film surface was observed when deposition was interrupted.

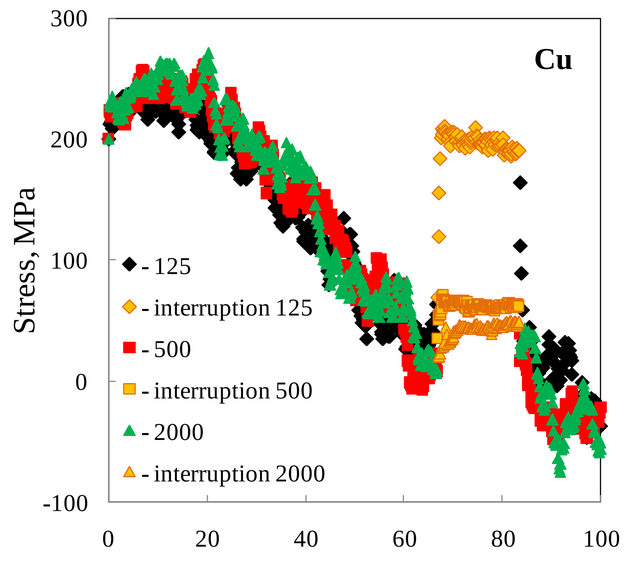
• Displacement vectors of atoms during deposition interruption and a graph of the distribution of their vertical components. Vectors of small displacements became points.



Effect of temperature and deposition rate on stress relaxation



• Evolution of stress in Cu films during deposition with an energy of 15 eV at temperatures of 300 K and 500 K.



• Evolution of stress in Cu films during deposition with an energy of 15 eV at deposition rate 125, 500 and 2000 steps.

Conclusions

1. The results of MD simulation show that the reversible relaxation of compressive stress in polycrystalline films upon interruption of deposition is associated with the redistribution of atoms within grain boundaries. The atoms are redistributed laterally, resulting in a more compact arrangement.

2. The process of rearrangement of atoms in the grain boundaries proceeds in the same way in all layers of the film, not only after the deposition has stopped, but also during it.

3. The higher the mobility of atoms on the surface, the greater the change in stress upon interruption of deposition.

4. The higher the film deposition rate, the greater the change in stress when deposition is stopped.

5. No escape of atoms back to the film surface upon interruption of deposition was observed.

References:

[1] S. Plimpton. J. Comput. Phys., 117 (1), 1 (1995). DOI: 10.1006/jcph.1995.1039
[2] A. Stukowski. Modelling and simulation in materials science and engineering, 18 (1), 015012 (2009). DOI: 10.1088/0965-0393/18/1/015012
[3] P. Jagtap, E. Chason. Acta Materialia, 193, 202 (2020). DOI: 10.1016/j.actamat.2020.04.013

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