Molecular-dynamic study of processes at the interface of a flat metal heterostructure during its heating

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Abstract. The author applies the method of heating to a flat copper-silver heterostructure. An approach has been developed for carrying out a meso-analysis: the study of the distribution of parameters such as temperature, concentration of atoms, etc. in the direction perpendicular to the interface. A parameter describing the diffusion of atoms across the interface during heating has been proposed and calculated.

1. Introduction
In recent years, interest to the molecular-dynamic modeling of alloy formation on the atomic level has been rising.

In particular, analysis of phenomena in crystals during heating is of high interest [1]. As the alloy forms, the material interface occurs. A number of works [2–6] are devoted to the investigation of the phenomena on the crystal interface (either on grain boundaries, or the substrate and thin-film coatings).

However, our paper concentrates on the analysis of the physics of the processes at alloy formation, not only on the research of thermophysical proportion of the ready system resulting from the interface melting, which is a fundamental difference from the available works of other teams. The investigation type is close to the project group [7, 8].

Thus, this work is a pilot one in the field of the development of the physical and mathematical model of alloy formation, which would permit performing on the micro-level the detailed investigation of the influence of rates of thermophysical parameters of the matrix and nanocluster materials, as well as the external controlled parameters on the physical properties of the resultant alloys.

2. Physical system, initial data assignment
We set separately a silver crystal, a copper crystal, each shaped as a rectangular parallelepiped with the atoms located in the nods of a perfect FCC lattice. The sizes of sub-systems by the contact area and the interface are determined with due regard to the fact that the size of the crystal lattice constant for copper is smaller than for silver. The copper crystal lattice constant $a_{\text{Cu}} = 3.615$ Å; the silver crystal lattice constant $a_{\text{Ag}} = 4.09$ Å. We choose the sizes on the heterostructure base, regarding the previous investigation about the effect of the chosen nano-object size on the calculation results [9].

Finally, the following sizes of the heterostructure components have been chosen: $n_x=30$, $n_y=10$, $n_z=5$ (7046 atoms of copper) for the copper part; $n_x=26$, $n_y=9$, $n_z=4$ (4532 atoms of silver) for the silver part. After that, in an individual software program, we place one part above the other within the distance of a half of the copper crystal lattice.
The Verlet velocity modification [10] was used for all further calculations, the time step $\tau = 10^{-16}$ s. Atomic interaction is calculated by the embedded atom method [11] with due regard to the composition: Cu-Cu, Ag-Ag, Cu-Ag.

3. Preparation of the physical system

Now, the resultant heterostructure should be cooled, to put it in the equilibrium state. This is done by the artificial viscosity method [12]. After 1 million of computational steps, the system gets into the energy global minimum condition with a slight atomic shift about the perfect crystal structure owning to the stress occurring at the interface; the stress is caused by the constant difference in copper and silver crystal lattices (figure 1). Then, the atom coordinates and momentums in this cooled heterostructure are used as the initial data.

![Figure 1. Outlook of the cooled Cu-Ag heterostructure.](image)

4. Heterostructure heating

The heating procedure is carried out with the stochastic impulses method [13]. Figure 2 shows the main calculated characteristics.

The link energy is calculated as the difference of the full system energy and energies of the copper and silver sub-systems and corresponds to the energy, which is needed to split the heterostructure by the sub-systems and separate them infinitely:

$$U_b = U_t - (U_{Cu} + U_{Ag})$$

The figures below show the heated heterostructure at different temperatures (figures 3 and 4).

It is evident that at $T = 1100$ K (figure 4), which is close to the silver melting point, the systems begin to bend. This results from two factors: weakening bindings between atoms during the heating and difference between the constants of copper and silver crystal lattices.
Figure 2. Energy characteristics versus the time step during the heterostructure heating. (a) the whole system temperature; (b) the heterostructure full energy; (c) the kinetic energy of heterostructure atoms (minus the energy of motion of the heterostructure mass center); (d) the varying energy of link between silver and copper parts; (e) the potential energy of the copper part; (f) the variation of the internal system energy.

Figure 3. Outlook of the heterostructure in the XZ plane at T=100 K (a) and T=300 K (b).
At 1300 K (which is close to the copper melting point and above the silver melting point), the heterostructure loses its initial rectangular-parallelepiped shape and tends to the spherical shape.

![Figure 4](image_url)

**Figure 4.** Outlook of the heterostructure in the XZ plane at T=1100 K (a) and T=1300 K (b).

5. Mesoanalysis

The system characteristics have been meso-analyzed at different temperatures, in order to see the dynamical changes of some parameters, which characterize the presence of diffusion through the interface. The mesoanalysis is realized via the mental splitting of the heterostructure to meso-cells by the planes parallel to the interface and perpendicular to the Z axis (in this task statement).

The coordinate \( Z_{\text{int}} \) of the copper-silver interface has been selected at the initial time instant (before heating) – and is shown by a straight grey line in the graphs below. The spatial step is equal to the half of the copper crystal lattice constant \( a_{\text{Cu}}/2 \). The size of the mesoanalysis domain is assigned in such a way to take the thermal dilation of metals into account.

The temperature distribution over the meso-cells along the Z axis has been studied, as well as the distribution of the relative amount of copper and silver atoms. We calculate the relative amount of atoms of the certain substance (copper or silver in this task) as the relation of this substance atoms amount in the selected meso-cell at the certain temperature to the amount of atoms of the same substance in the perfect cooled heterostructure:

\[
N_{\text{rel,Cu}}^i = \frac{N_{\text{mes,Cu}}^i(T)}{N_{\text{mes,Cu}}^i(T = 0)}; \quad N_{\text{rel,Ag}}^i = \frac{N_{\text{mes,Ag}}^i(T)}{N_{\text{mes,Ag}}^i(T = 0)}
\]

The “beak” in figure 5 (a) results from the fact that the meso-cell partition is connected with the copper crystal lattice constant, so at such a partition, some meso-cells get much fewer atoms than the other. In future, it can be excluded via increasing the meso-cell and physical system size. The fact that the copper sub-system temperature is higher than the one of the silver sub-system also proves that during the heterostructure heating, the time interval for the system relaxation to the equilibrium state should be increased as compared to the numerical heating of homogeneous systems. It is seen that, as the system is heated, the distribution of the relative amount of atoms perpendicularly to the interface becomes smooth, the breach disappears, which indicates the beginning diffusion of copper and silver atoms through the interface (figures 5 and 6).
Figure 5. (a) Distribution of the relative amount of Cu atoms (black dots) and Ag atoms (grey dots) perpendicularly to the interface. (b) Temperature profile at the copper-silver interface. The average heterostructure temperature $T=300$ K.

Figure 6. (a) Distribution of the relative amount of Cu atoms (black dots) and Ag atoms (grey dots) perpendicularly to the interface. (b) Temperature profile at the copper-silver interface. The average heterostructure temperature $T=1300$ K.
6. Conclusions
To model the heating of the flat heterostructure, more time should be given for the whole system relaxation to its equilibrium state at each temperature increase step. In our case, 600 steps were chosen ($10^{16}$ s or 0.001 in the computational measurement units), which was enough for the uniform system consisting of one substance atoms, but this amount should be increased for the heterostructure.

It is demonstrated that the meso-cell distribution of the relative amount of atoms perpendicular to the heterostructure interface (along the Z axis) can be used as the first sign of the atom diffusion through the interface.

The peaks on the dependence of the relative amount of atoms in the computational mesoanalysis cell result from the smallness of the whole system and, hence, small sizes of the meso-cells.

It is better to use the parameter obtained in the task of the spherical heterostructure as the criterion of diffusion presence: the relation of amount of atoms of the certain substance in the meso-layer at the certain temperature to the full amount of atoms in the same meso-layer at the same temperature T. The characteristics are smoother, without dramatic drops as in the case of meso-analysis, at the diffusion in the flat heterostructure, as the relation was found in respect to the amount of atoms of the same substance at the zero temperature.

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