Molecular-dynamic analysis of the strength change through absorption for metal nano-structures during the interaction with a metal melt

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Abstract. The present work is addressed to the development of the technique of calculation of the strength change for the metal samples under external loadings by the molecular-dynamics method. Such a strength change results from the absorption interaction with a metal melt on the nano-structure surface (a kind of the Rebinder effect). The timeliness of this problem is associated with the creation of the optimal technology of formation and processing of structural materials for up-to-date equipment. The paper presents the developed approaches to the Rebinder effect simulation by the molecular-dynamics method. The influence of a melted silver drop on a copper surface on mechanical characteristics and general geometry of the system under the action of the tension stress is studied by means of comparison with the copper sample under the action of the same tension stress.

1. Introduction

It has been found experimentally that the interaction between a melted metal (or another liquid medium, for example, acid) and metal in the solid phase results in the strength reduction of the metal sample which is initially in the stressed condition. Such conditions may occur during the performance of metal structures in natural conditions. The melt contacts solid-phase metal, for example, during the welding in the Arctic, or in external constructions in orbital stations at very low temperatures.

The absorption strength reduction of metal structures under external loadings which appears as the result of the physical and chemical action of the medium on these structures (the Rebinder effect) has been attracting serious attention for about 90 years. Detailed analysis and multiple kinds of this effect are presented in many works, for example in [1].

As computational equipment progressed, the works of Rebinder followers contain the results of numerical investigation of the absorption reduction of material strength, for example [2]. However, inadequate computational equipment restricted the variety of considered effects by the simulation in 2D systems.

In two recent decades, only one work [3] on this topic stands out. It considers the interface of the solid crystal Al and liquid Al, analyzes the effect of the discrepancy of their crystal lattices. In spite of the fact that the physical system used is similar to the one to be considered herein, the authors of [3] do not study the Rebinder effect at all.
Thus, the main purpose of this work is the molecular-dynamic analysis of mechanical damages of the metal samples under the action of the external loadings resulting from the absorption interaction with a melted metal.

2. Ideas of methodology of the Rebinder effect analysis
The major problem stated by Rebinder and his followers is the construction of the atomic model of the absorption strength reduction (ASR) for the metal structures already under external loadings. This work focuses all attention on this effect but it results solely from the interaction between the melted metal and solid-structure surface.

Hence the initially stated task requires the following sequence of operations. At the initial time instant, there is a solid metal structure in the equilibrium thermodynamic and statically stressed condition. A drop of another metal forms on the surface of the first structure, the other metal is melted. After that, the characteristics of transition processes of this system into the stationary and statically equilibrium state is studied.

At the first stage, the calculation of the dynamics of the processes in the solid-state system with the perfect crystal structure without any defects, which forms under the action of controlled external disturbances are performed as the standard. The results of this stage can be proven by multiple experimental and numerical data available today.

At the second stage, the system from a melted metal drop is formed on the surface of the same system in the undisturbed condition; the procedure of the first-stage loading is repeated. Obtained differences in the results show which characteristics are influenced by the melted metal drop and how they are influenced.

3. Analysis of the effect of a liquid metal drop on the perfect structure
The work presents the numerical experiment of the effect of a liquid metal drop on the tensile dynamics of a copper parallelepiped under the action of the constant tensile axial stress. Then we present the results for the tension stress of 5GPa. Silver was used as a melted metal. The numerical experiment was carried out when the temperature of the copper brick was below 5K, the silver drop temperature was about 1,500K. All numerical experiments were carried out within the time range below 300 ps.

To simulate the tension of the lower brick (with or without melted silver drop), the following clamps were used: the atoms of the leftmost atomic plane of the copper parallelepiped perpendicular to the X axis were fixed in the 3D biharmonic potential to simulate the immovable clamp.

Simulation of the movable clamp in this work was done as follows: basing on the preset external stress and area of the right edge (which was re-calculated during the sample tension), we find the total external force acting on the system. Since we know the number of atoms on this edge, we can calculate the force acting on each atom.

In the work we used the Verlet velocity modification of the second order of accuracy [4] with the time step $10^{-16}$ s. In the case of the isolated system, the energy error does not exceed $10^{-5}$ % in the time range of 50 ps.

3.1. Simulation of the initial state of the copper parallelepiped with the perfect crystal lattice
The paper presents the results for the rectangular parallelepiped with the following number of crystal cells $n_x = 17, n_y = 7, n_z = 5$ along respective axes of coordinates. To simulate the interaction between atoms, we used the potential construed on the embedded atom method base [5]. Then the structure was cooled down by the artificial viscosity method [6], and the position of the atoms in the global minimum of the potential energy was determined.

The second structure with this geometry of the copper parallelepiped was prepared in accordance with the version of the silver drop on the surface as follows: initially, the parallelepiped was formed from silver atoms, the crystal cell sizes $n_x = 10, n_y = 3, n_z = 3$ along the respective axes. Then the brick
was cooled down to cryogenic temperatures and was located above the already cooled copper structure (its sizes \( n_x = 17, n_y = 7, n_z = 5 \)) within the distance of \( \Delta z = 4.09 \) Å. Then the silver structure was cooled again in the copper atoms field. The copper atoms were excluded from the motion equations. It permitted optimizing interatomic distances in the system under the condition of the minimal total energy.

Then the silver structure is heated up to the temperature about 2,000K. The heating was done by the method developed in [7]. The fundamental difference of the heating in this work is that only the silver subsystem was heated, but the silver atoms were located in the stationary field of copper atoms. As a result, the temperature of copper substrate was constant and equal to \( 0.519 \cdot 10^{-4} \)K. Figure 1 presents the position of the atoms of the system after silver heating up to 1,520.25K.

3.2. Methodology of simulation of isothermal tension of the two-component structure
The most convincing way is to compare the dependence of main characteristics of the copper brick on time for two versions: without melted silver drop and with the melted silver on the surface. The stress dependence on the movable clamp on time is described by the Heaviside function. Below there is the illustration for the process in which the temperature was not corrected, i.e. the heat exchange between the silver drop (1,520.25K) and copper substrate \( (0.519 \cdot 10^{-4} \)K) took place. Figure 2-a shows that there is the strong heat exchange between the components, and, by the 20 ps, the average temperatures are leveled and fluctuated around 500K. The other paradox is that the relative elongation of the copper component took the constant value around 60% (Figure 2- b) by the time instant of 40ps.

The structure outlook shows that the silver drop extended over the copper sample, the whole system becomes more plastic at 500K, and there is no rupture.
It means that the temperature adjustment is needed for the Rebinder effect simulation. At the moment of the tension of the system with the silver melt, certain quite small temperature deviations $\Delta T_{Cu}$, $\Delta T_{Ag}$ were assigned, and the copper and silver temperatures were checked at each time step. As soon as the copper temperature exceeded the preset value $T_{Cu} + \Delta T_{Cu}$, or the silver temperature got below the preset value $T_{Ag} - \Delta T_{Ag}$, farther time calculation was stopped, and the adjustment of the needed component temperature started [6]. After the recovery of the needed temperatures, the dynamics calculation was continued. Below there are the numerical results for the following extreme-deviation values: $\Delta T_{Cu} = 5 \, \hat{E}$, $\Delta T_{Ag} = 20 \, \hat{E}$. The copper component temperature is about 0K, the silver drop temperature is 1,500K.

3.3. Effects of the melted silver on the copper sample tension

Under the stress, a strong non-equilibrium process appears in the pure-copper sample, the temperature rises dramatically from 0K to 90K, and from about the 80 ps it starts decreasing smoothly. The copper temperature in the complex system is equal to 5K with the accuracy up to 0.01K. The lower boundary of the silver temperature is 1,500K, i.e., silver is always melted.

Figure 3 demonstrates the dependencies of the potential energy of both systems on time. Dramatic difference is seen in the behavior of these characteristics for the perfect copper rod and for the system with the silver melt. It is of special importance to note that the potential energies converge to one stationary value.

Figure 3. Potential energy versus time: the pure copper system (a); the copper component of the Rebinder system (b).

Equally essential difference is observed for the dependence of the relative deformation on time for these two systems. The value of the relative elongation of the structure with the silver drop is approximately three times lower than the same value for the perfect copper rod.

Below there is the synchronic illustration of the processes in the considered structures exemplified by the atom location in the XZ plane. By the 10 ps, multiple point translation defects began to form near the movable clamp of the perfect copper structure (Figure 4 a); at the same time, the almost-perfect crystal structure remains the same in the copper component of the Rebinder structure (Figure 4 b).

By the 30 ps, an accumulation of dislocations started to form near the movable clamp; this accumulation shifted toward the immovable clamp by the 100 ps. By this time, the copper component started bending slightly toward the silver drop (in the Rebinder system).

By the 300 ps, the oscillating shifts of the movable clamp become evident in the copper rod (Figure 5 a). At the same time, there are no dislocations in the Rebinder system, just a certain bend of the copper sub-system, and the silver drop expansion over the copper surface (Figure 5 b).

Hence, initially we have two absolutely similar objects: copper rectangular parallelepipeds with the perfect crystal lattice, but one has a drop of liquid silver on it. But, under the mechanical loading (tensile stress), under the external stress action, every characteristic of these objects differs
dramatically, as if we work with two completely different materials. Note that the copper rod with the silver drop demonstrates better strength properties.

Figure 4. Outlook of the comparative systems in the XZ planes at 10 ps. (a) the copper system; (b) the system of copper and melted silver drop. Black bubbles are copper atoms, grey bubbles are silver atoms.

Figure 5. Outlook of the compared systems in the XZ planes at the time instant 300 ps. (a) the copper system; (b) the system of copper and melted silver drop. Black bubbles are copper atoms, grey bubbles are silver atoms.

4. Conclusion
The numerical analysis on the atomic level shows that the liquid silver deposited on the surface of the copper rod causes the effect of absorption strength changing. The difference from the Rebinder effect lies in the absorption strength amplification for the used initial parameters of the system.

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