MOLECULAR DYNAMICS STUDY OF THERMAL HYSTERESIS DURING MELTING-CRYSTALLIZATION OF NOBLE METALS

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Summary. By constructing the thermal hysteresis of the enthalpy and density of the noble metals of gold (Au) and copper (Cu), non-equilibrium processes are investigated during the melting – crystallization phase transformations, i.e. during the solid–liquid transition. Thermal hysteresis is obtained from the atomistic modeling. The limiting temperatures of superheating of the solid phase during melting and undercooling of the liquid phase during crystallization of gold and copper are obtained. The possibility of the formation of highly superheated-undercooled metastable states of solid and liquid phases with rapid heating-cooling of the studied metals has been confirmed. The results obtained are compared with the results of alternative calculations.

1 INTRODUCTION

The phenomenon of melting-crystallization of metals, which is a phase transformation of the first kind, plays an important role in materials science and engineering. In recent years, extensive experimental [1-10] and theoretical studies combined with modeling of melting-crystallization of solids [11-21] have significantly expanded the understanding of the nature of this phenomenon. The processes of melting-crystallization proceeding in a quasi-equilibrium way are the most studied [22,23,24]. The trajectory of melting-crystallization processes in phase space passes through the equilibrium states only in the extreme case of infinitely slow heating/cooling. In this case, the temperatures of the beginning and end of melting, as well as the beginning and end of crystallization, will coincide both with each other and with the equilibrium melting temperature. Changing the heating regimes of the target can lead to a non-equilibrium behavior of the melting – crystallization processes, manifested in the phenomenon of thermal hysteresis. Thermal hysteresis is characterized by a mismatch of melting and crystallization temperatures, as well as thermodynamic characteristics of the material (enthalpy, density) during heating and cooling. The study of thermal hysteresis has been carried out by many researchers both experimentally [1-4] and theoretically [17-21]. The studies were carried out mainly to analyze the dimensional effect and the influence of the interphase structure on the melting processes [2,4,5,7,17,21], to study the degree of overheating-undercooling of metals [1-3,18-20], the influence of thermal hysteresis on the properties of metals [2,17,18].

One of the regimes of thermal action, in which the phenomenon of thermal hysteresis of metals occurs, is the rapid action of powerful concentrated energy flows on the target. Under such influence, the melting-crystallization processes become non-equilibrium, and phase transitions are accompanied by the appearance of metastable superheated-undercooled states

in the initial phase [20,25]. The magnitude of thermal hysteresis, being a characteristic of the degree of superheating-undercooling of the condensed phase, is related to the velocity of the phase front [12, 26]. The magnitude of energy costs during the destruction of long-range bonds during melting gives an idea of the degree of non-equilibrium of the melting process. Therefore, the hysteresis properties are of significant interest for the study of non-equilibrium melting-crystallization. The study of this phenomenon also contributes to solving such a fundamental problem as determining the limit values of superheating of a solid and undercooling of a liquid. The experimental approach to the study of thermal hysteresis of materials, which is traditional, has a number of limitations, primarily in the range of measurement conditions, especially in the melting region. It is known that experiments on the study of undercooling of metals [10] are well described in the literature, in contrast to studies of superheating. Because of this, it is relevant to use the theoretical approach [11-17, 19-21, 26, 27] in the study of melting-crystallization processes, the main tool of which is the method of molecular dynamics (MD).

This article discusses the features of non-equilibrium melting and crystallization of noble metals of gold and copper based on thermal hysteresis of enthalpy and density in the temperature range $0.60 \leq T \leq 2.00$ kK. Thermal hysteresis is obtained for the metals under study from the molecular dynamic modeling. The potentials from the "embedded atom method" (EAM) group developed and tested in [27] for gold and in [28] for copper were used as interparticle interaction potentials.

2 METHODS AND APPROACHES

In this paper, the thermal hysteresis of enthalpy and density for gold and copper is obtained based on an atomistic approach. The method of molecular dynamics (MD) has become widely used for the numerical solution of atomistic models. The atomistic approach is based on a model representation of a polyatomic molecular system in which all atoms are represented by material points whose motion is described by classical Newton equations. Atomistic models are a system of differential equations, for the integration of which initial conditions are set in the form of values of coordinates and velocities of all particles at the initial time t = 0. The resulting system of ODE is solved using the finite-difference Verlet scheme [29].

In MD modeling, the choice of the interaction potential between the particles plays an important role, since the reliability of the results obtained directly depends on it. To model the properties of the metals under consideration, the potentials from the EAM group were used, developed and tested for gold in [27], for copper in [28], allowing for a good description of both the crystalline and liquid phases of the metals under study.

For both metals, the simulation was carried out in the temperature range $0.60 \leq T \leq 2.00$ kK using the widespread LAMMPS package (large-scale atomic-molecular massively parallel simulator) [30]. It implements support for many paired and multiparticle short-range potentials, the ability to record atomic configurations in a text file, and also has built-in thermostats and barostats. The temperature and pressure for the ensemble of particles were regulated using a thermostat and a Berendsen's barostat [31].

In this paper, the enthalpy and density of metals in an isobaric heating and cooling process involving phase transitions were determined from a series of molecular dynamic calculations within the framework of a single computational experiment. The computational experiments planned in a similar way were carried out for both metals. The calculated area was selected in

the form of a cube, with dimensions of 30×30×30 elementary cells, containing a FCC crystal of 108,000 particles. Periodic boundary conditions were set in all directions. The particle velocities were set in accordance with the Maxwell distribution at a temperature of 0.60 kK. The relaxation procedure preceding the simulation was carried out at a temperature of 0.30 kK and zero pressure. Next, the sample was heated at a constant rate of approximately $V \sim 0.56 \times 10^{12}$ K/s. Heating continues to a temperature of 2.0 kK, at which the sample was completely melted, which made it possible to record the temperature dependences of density ρ (T) and enthalpy $H(T)$ during heating. At the same time, the sample was prepared for cooling and subsequent registration of the dependences of density ρ (T) and enthalpy $H(T)$ during cooling. Cooling, as well as heating, of the sample was carried out at the same constant speed V. The experiments were carried out at a constant zero pressure $P = 0$.

During modeling of the changes in a condensed medium, it is important to distinguish its aggregate state due to long-range and short-range bonds. The order parameter can be used as a criterion for this. In order to distinguish the type of ordering during the melting-crystallization phase transition, the order parameter of the heating and cooling was obtained for copper and gold. The approaches to determining the order parameter used in this paper are presented in [32].

3   MODELING RESULTS

The results of MD modeling are presented in Fig.1-4. Fig.1(a,b) shows the thermal hysteresis loops of the enthalpy of gold and copper, which are represented by the generally accepted values of the increment $\Delta H(T) = H(T) - H(0.298°\text{kK})$. The hysteresis of the density of copper and gold is shown in Fig.2 (a,b). Figure 3.4 shows the order parameter for the heating and cooling of copper and gold. The vertical dotted lines in all figures indicate the equilibrium melting point, which for gold is Tm = 1.332 kK, for copper – Tm = 1.33 kK. These values of the equilibrium melting point of copper and gold are obtained from molecular dynamic calculations [33, 34] using the potentials [27,28]. The reference values [35] of the equilibrium melting point are for gold T_m=1337 K and copper T_m=1356 K. The difference between the reference values and the obtained values for gold was $\Delta T_m = 0.38\%$ and for copper $\Delta T_m = 1.96\%$. The error is quite acceptable for modeling.

Figures 1, 2 also show the temperature of the end of crystallization T_{cr}, the limit temperatures of superheating of the solid phase T^+ and supercooling of the liquid phase T, which are the temperatures of the beginning of melting and the beginning of crystallization, respectively. These temperatures determine the vertices of the hysteresis contour, which in Figures 1, 2 is indicated by the letters ABCDEF.

The thermal hysteresis loops (Fig. 1,2) are formed when the heating (red) and cooling (blue) curves are combined, taking into account the forward (melting) and reverse (crystallization) phase transitions. The directions of the heating and cooling processes are shown in Figures 1,2 with arrows. In the considered temperature range, the heating of copper and gold occurs with the absorption of heat (endoprocess), which is expressed in the superheating of the solid phase. The most important characteristic of the stability limit of the crystal lattice is the limit temperature of superheating of the solid phase T^+. The maximum superheating temperatures of gold and copper, normalized by the corresponding equilibrium melting temperatures T_m, are shown in Table 1.

	Heating			Cooling			Ref. [20]				Ref. [37]
	T_m [kK]	T^+	θ^+	T_{cr} [kK]	T^-	θ^-	θ^+_{md}	θ^+_{ns}	θ^-_{md}	θ^-_{ns}	θ^+_{ns}
Au	1.332	$1.235T_m$	0.235	0.983	$0.589T_m$	0.354	0.3	0.2	0.44	0.25	0.184
Cu	1.33	$1.203T_m$	0.203	0.975	$0.603T_m$	0.357	0.21	0.19	0.3	0.24	0.174

Table 1. Heating-cooling properties of gold and copper.

As one can see, the value of superheating in gold is slightly higher than in copper. Upon reaching the temperature T^+ (point B in the hysteresis contour in Fig. 1, 2), a superheated metastable state of the solid phase begins to form, which is characterized by the beginning of the formation of stable nuclei of the liquid phase and intensive destruction of the crystal lattice. Therefore, the temperature of the ultimate overheating T^+ is the temperature of the beginning of melting. The formation of a metastable state in both gold and copper is accompanied by a further drop in the density of the solid phase (Fig. 2). During the melting process, in the temperature range $T_m < T < T^+$ (line BC of the hysteresis contour in Fig.1, 2), part of the kinetic energy of the chaotic motion of particles is spent on the destruction of the crystal lattice. The temperature of the end of melting (Fig. 1, Fig.2) in our calculation, at the heating rate $V \sim 0.56 \times 10^9$ kK/s, it practically coincides with the equilibrium melting point of each of the metals T_m. At a higher heating rate, the difference between these temperatures can be significant [36,37]. With further heating, the thermal expansion of the liquid occurs. Relative overheating of the solid phase $\theta^+ = (T^+ - T_m)/T_m$, which is observed in the enthalpy hysteresis (Fig.1) and the densities (Fig.2) of the metals under study are given in Table 1. For gold $\theta^+ \approx 0.235$, for copper – $\theta^+ \approx 0.203$. In [20], the values of relative overheating of gold $\theta^+_{md} \approx 0.3$ (md index) and copper $\theta^+_{md} \approx 0.21$ were obtained from MD calculations with a heating rate $V = 10^9$ kK/s and calculated using the classical theory of homogeneous nucleation (ns - nucleation in the solid phase) for gold $\theta^+_{ns} \approx 0.2$, for copper $\theta^+_{ns} \approx 0.19$. In [38], the values of the relative overheating of the solid phase of copper $\theta^+_{ns} \approx 0.174$ and gold $\theta^+_{ns} \approx 0.184$ were also obtained. Comparison of the obtained results with the results of alternative calculations [20, 38] shows a good correspondence. According to estimates [17, 20], metals can be superheated to the temperature of the beginning of a massive homogeneous transformation $T^+ \approx 1.3T_m$, which is also consistent with the results for the metals studied in this work.

The melting phase transition at a temperature of $\sim T_m$ for gold and copper (see Table 1) is clearly identified by a large difference in the enthalpies of the liquid and solid phases, representing the specific heat of melting L_m of the metals under study. According to the results of calculations, the specific heat of melting for gold is $L_m \approx 12.39$ kJ/mol, or 43.14%, for copper – $L_m \approx 12.05$ kJ/mol, or 41.46% (Fig.1). The increase in enthalpy is accompanied by a decrease in density, while the difference in density of the liquid and solid phases is for gold $\Delta\rho_{melt}(T_{sl}) \approx 6\%$, and for copper $\Delta\rho_{melt}(T_{sl}) \approx 4.8\%$ (Fig.2 (a,b)). The temperature dependences of the order parameter of copper and gold during heating are shown in Fig.3 (a, b). With increased heating, the order parameters of the solid phase decrease until the maximum temperature of superheating $T^+ > T_m$ is reached, resulting in the destruction of the crystal lattice and intensive nucleation of the liquid phase. At a temperature close to T_m, the order parameter decreases sharply to almost zero, confirming the transformation of a metal

crystal into a liquid. As one can see, during the phase transition of the 1st kind, the order parameter changes abruptly.
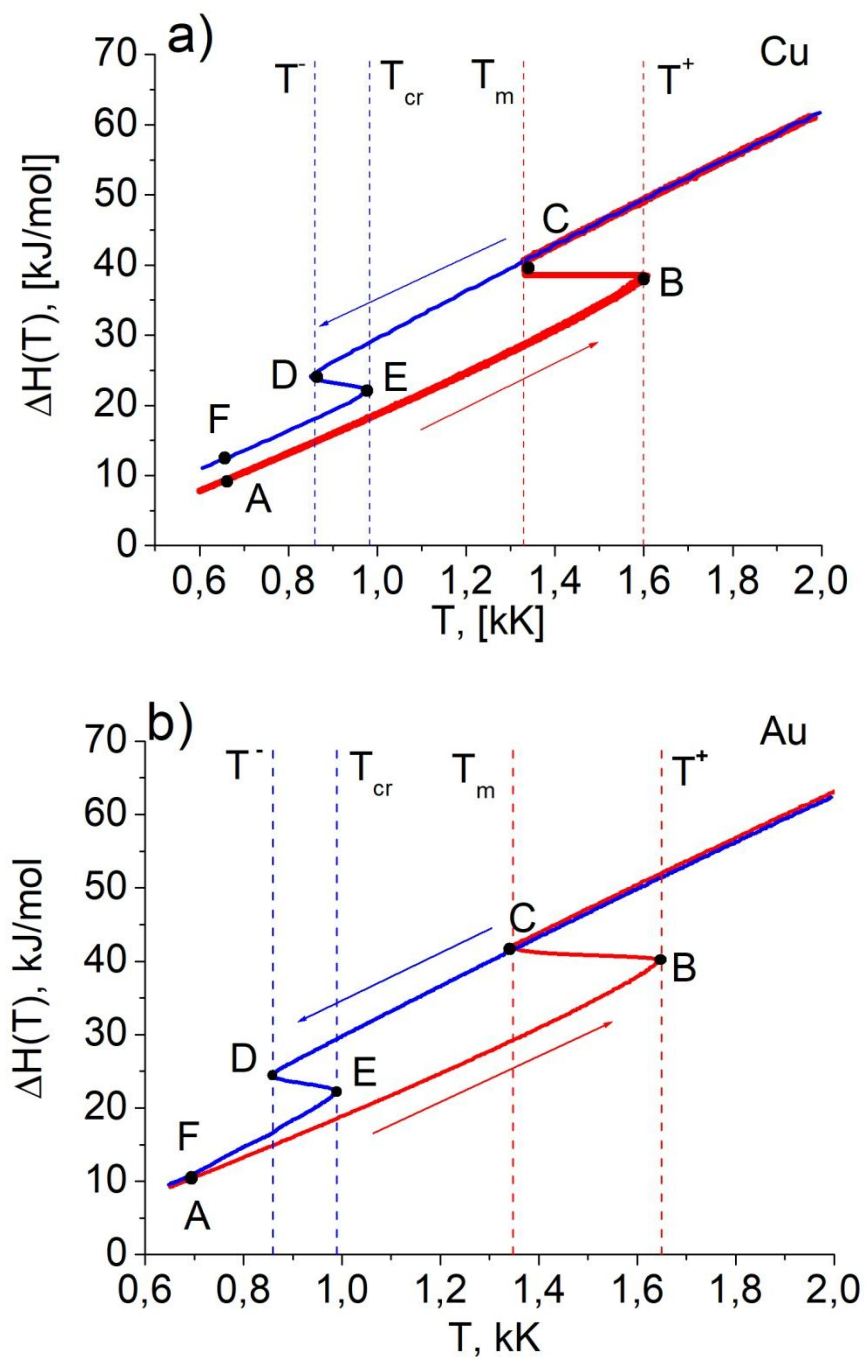

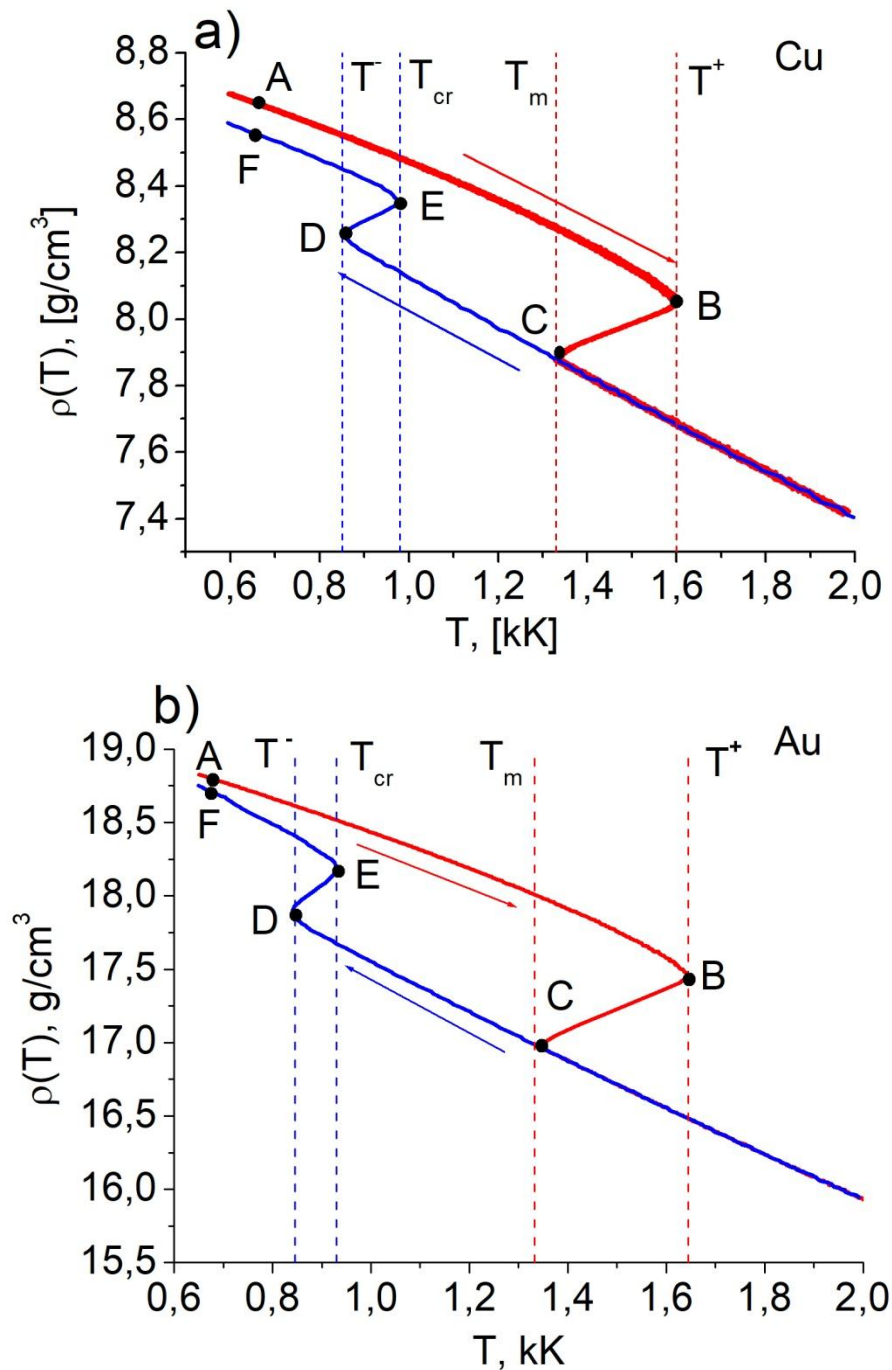Fig. 1. Themal hysteresis of enthalpy for a) copper, b) gold.

Fig. 2. Thermal hysteresis of density for a) copper, b) gold.

Cooling of copper and gold targets, unlike heating, occurs with the release of heat and is an isoprocess. Crystallization turns out to be much more sensitive to the cooling rate. The ultimate undercooling temperature T of the liquid phase, normalized to the melting point T_m, for gold and copper is shown in Table 1. The ultimate temperature of undercooling is the temperature of the beginning of crystallization, at which the formation of the first stable

nuclei of a new solid phase occurs. On the segment DE of the hysteresis contour (Fig. 1,2), there is a rapid growth of the formed nuclei of the new phase due to the rapid movement of their boundaries along the undercooled liquid phase, representing the crystallization fronts. In this case, the crystallization fronts are always undercooled relative to the equilibrium melting temperature T_m. At the point E (temperature T_{cr}), the liquid phase completely disappears.
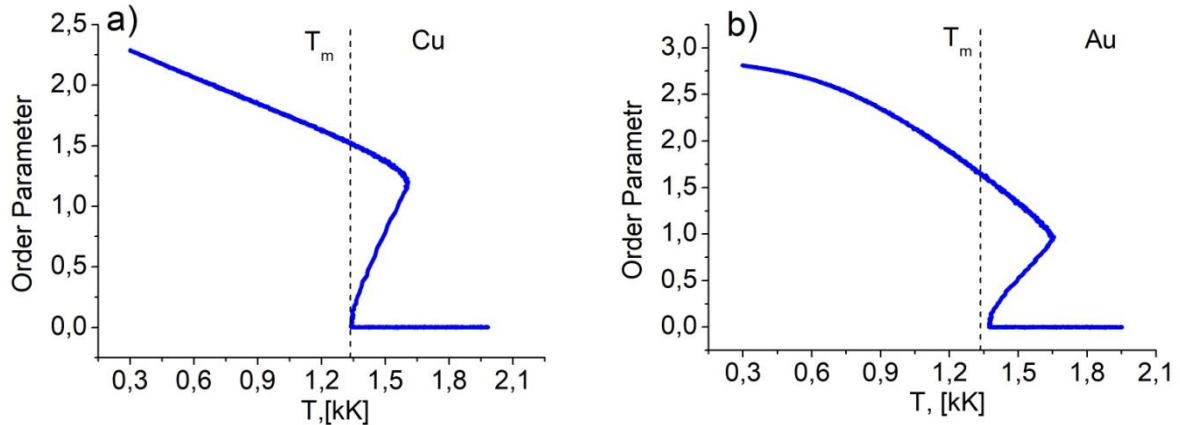

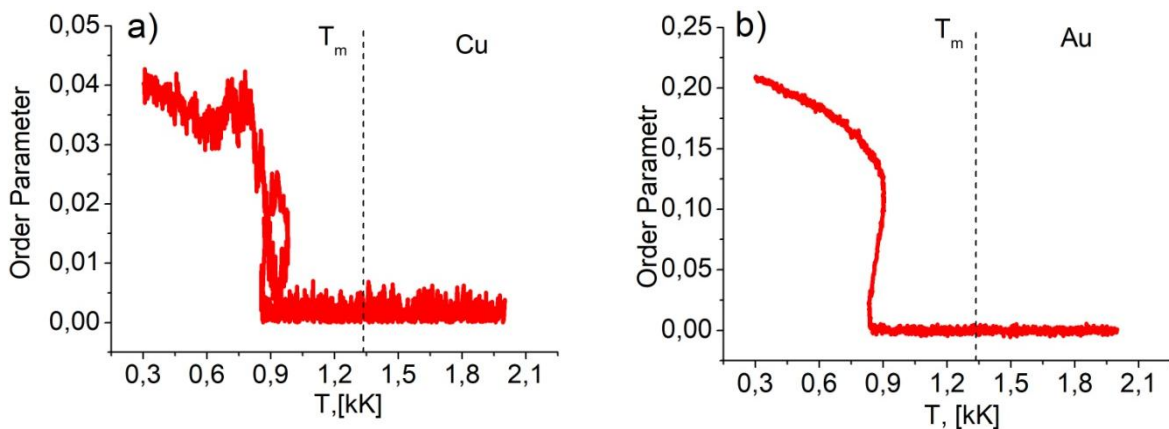Fig. 3. Order parameter during heaitng of a) copper и b) gold.

Fig. 4. Order parameter during cooling of a) copper и b) gold.

The end of crystallization occurs at the T_{cr} temperature given for copper and gold in Table 1 (point E in the hysteresis contour in Fig. 1, 2). In our calculation, due to the high cooling rate $V \sim 0.56 \times 10^9$ kK/s, the crystallization termination temperature T_{cr} is lower than the equilibrium melting temperature T_m, by $T_m - T_{cr} = 0.355$ kK for copper, and by $T_m - T_{cr} = 0.349$ kK for gold. Too high cooling rate in our calculation led to the fact that the density of the substance at the T_{cr} temperature turned out to be less by 1.7% in gold and 1.51% in copper than the density of the crystal when heated. The density of the new phase despite the constant increase of it (line EF in Fig. 2) remains less than the crystalline one (the line AB of the hysteresis contour in Fig. 2). This discrepancy is especially noticeable in copper, where the density of the new phase is less than the crystalline one at $T = 0.6$ kK by 1.06%, whereas in gold this difference is only 0.355%. Figure 4 (a) shows the temperature dependence of the

order parameter during cooling for copper. The order parameter of copper during cooling is by ~98.2% less than the order parameter of the crystal during heating (Fig. 3(a)), which indicates a strong undercooling of the melt, in which non-crystalline types of the solid phase (vitrification or amorphization) are realized. The order parameter of gold during cooling (Fig. 4 (b)) is about 10 times less than the order parameter of the crystal during heating (Fig. 3 (b)), which also indicates, although to a lesser extent, a strong undercooling of the melt and the formation of non-crystalline solid phase species.

Relative undercooling of the liquid phase $\theta^- = (T_m - T)/T_m$, which is observed in the enthalpy hysteresis (Fig.1) and densities (Fig.2), according to the results of MD modeling for gold and copper are presented in Table 1. Comparison with the results [20] obtained from MD calculations and from calculations using the classical theory of homogeneous nucleation, are respectively for copper $\theta^-_{md} \approx 0.3$, $\theta^-_{ns} \approx 0.24$ and for gold $\theta^-_{md} \approx 0.44$, $\theta^-_{ns} \approx 0.25$, which shows a good agreement with the presented results.

The maximum hysteresis value in this work was for gold $\Delta T_{Hyst} = T^+ - T \approx 0.589 T_m$ and for copper $\Delta T_{Hyst} = T^+ - T \approx 0.56 Tm$, which is consistent with the estimate of the hysteresis width for metals of $0.66 T_m$ [17].

The resulting thermal hysteresis of enthalpy and density, as well as the order parameter for heating and cooling of gold and copper, demonstrate the formation of metastable regions and the non-equilibrium nature of melting-crystallization processes.

4.   CONCLUSIONS

The hysteresis of the enthalpy and density of gold and copper in the range of 0.6 kK ≤ T ≤ 2.0 kK was obtained from a series of molecular dynamic calculations within the framework of one computational experiment. The resulting hysteresis demonstrates the formation of metastable regions and the nonequilibrium nature of the melting-crystallization processes of the studied noble metals. The analysis of the thermal hysteresis value at the heating and cooling rate $V \sim 0.56 \times 10^{12}$ K/s allowed us to estimate the degree of superheating-undercooling of the condensed phase. The obtained limit temperature of superheating of the metastable state of the solid phase and relative superheating, as well as the limit temperature of undercooling and relative undercooling of the liquid phase of both metals are in good agreement with the results of alternative calculations [17,20,38]. The maximum hysteresis value for gold $\Delta T_{Hyst} \approx 0.589 T_m$, for copper $\Delta T_{Hyst} \approx 0.56 T_m$ is consistent with the estimate of the hysteresis width for metals of $0.66 T_m$ [17].

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