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Mechanism of the formation of the structure and phase state of binary metallic nanoparticles obtained by the electric explosion of two wires made of different metals

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ABSTRACT

Based on the statistical approach to the description of the structure of liquid metals, it has been shown that during wire heating with a current pulse, the drastic local increase in the electric resistance of the liquid metal leads to the development of overheating instability. The increase in the electric resistance of the liquid metal is a consequence of the destruction of individual atom clusters that form short range order in the liquid metal. Non-uniform heating leads to the transition of liquid metal into a two-phase "gas-liquid" state formed by the expanding products of the explosion of wires. The majority of the expanding wire explosion products are liquid phase particles; those coagulate to form a binary melt. It has been shown by the example of Pb/Al, Ag/Cu and Cu/Al nanoparticles forming during the electric explosion of two wires made of different metals that the structure and phase state of the particles is determined by the probability of the formation of the binary melt that depends on the temperature of the coagulating particles.

1. Introduction

The electric explosion of wires (EEW) is used for the following purposes: research the state of matter under high-energy stress [1–12], generate shock waves and X-ray radiation [13,14], initiate a discharge channel [15], obtain nanoparticles of metals, alloys and chemical compounds [16–18]. Also, EEW can be used for obtaining binary nanoparticles of different metals by the electric explosion of two wires made of different metals [19–23]. However, the mechanism of the formation of the structure and phase state of the above particles remains unclear, because the physical processes taking place during the heating of wire with a pulse of current with the current density of $j > 10^7$ A/cm^2 are diverse and complex [1,2].

Binary nanoparticles formed during EEW have lognormal distribution by size which suggests that the nanoparticles are formed as a result of the coagulation of smaller particles [20]; these particles constitute the bulk part of the expanding products of the explosion [9]. However, a particle formation mechanism that would explain particle size and temperature has not been offered in scientific literature.

Authors of [24] conclude that the presence of particles in the expanding products of EEW is the consequence of non-equilibrium heating of the wire; the latter is caused by the fact that conduction electrons are mostly dissipated on the borders of grains/crystallites. According to the authors of [24], energy deposition on the borders of crystallites determines the direct dependence of nanoparticle size on the size of wire crystallites. As per [24], the suggested model of particle formation is in accordance with the cluster model of the structure of liquid metals based on the sustained existence of "dense" ordered areas in the liquid metal; the "dense" areas are separated from each other by areas with "sparse" unordered structure [25].

The research conducted in Ref. [26] has shown that an increase in the size of grains/crystallites of copper wire does not cause the average size of nanoparticles to increase. According to the data in Ref. [27], during EEW, in the liquid phases of the L63-zinc alloy couple, the electric resistance decreases as the temperature is increased, which cannot be explained by the cluster model of liquid metals structure. According to the cluster model, an increase in the temperature of a liquid metal leads to an increase in the volume ratio of the "sparse" structure, which results in the electric

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resistance increasing along with the temperature increase [25].

A decrease in the electric resistance of the liquid phases of the L63-zinc alloy couple with the temperature growth can be explained by the Ziman theory that is based on the statistical model of liquid metals structure [28]. According to the Ziman theory, electron scattering in a liquid metal/alloy formed in equilibrium heating conditions takes place at a weak chaotic potential that spans the entire volume of the liquid metal/alloy combination. The electric resistance of the liquid phases of the L63-zinc alloy couple that decreases along with the temperature growth demonstrates that in the course of wire heating by a pulse of current with the density of $j > 10^7$ A/cm^2 above the metal/alloy melting temperature, liquid metal/alloy is formed while the short range order (atom clusters) is preserved; this short range order is peculiar to the "solid-liquid" phase transition in equilibrium conditions.

In our opinion, the destruction of individual atomic clusters causes a drastic local increase in the electric resistance of the liquid metal, which leads to its non-uniform heating that promotes the formation of overheating instability throughout the volume of the wire [8]. Overheating instability are the main channel of energy dissipation, which leads to the destruction of the wire into liquid phase particles and gas/plasma that form the expanding products of the explosion [9].

Based on the statistical model of liquid metals structure, the present work is offering a mechanism of the formation of overheating instability in the conditions of EEW. This research estimates the values of minimal particle temperatures present in the expanding products of EEW; it also suggests a mechanism explaining the formation of the structure and phase state of binary particles obtained by the electric explosion of two wires made of different metals.

2. Theoretical model

The structure of the liquid metals was researched according to the cluster associate model [29]. The cluster associate model was developed for the purpose of researching the thermal dependence of the viscosity of liquid metals; the research was based on the statistical approach to describing the structure of liquids. The model was based on the Boltzmann distribution by melting and boiling thermal thresholds applied to atoms. According to the model, the atoms that are above the boiling point threshold develop a completely chaotic liquid state ("quasigas" dynamics), and the atoms below the boiling point threshold (those are referred to as "flowable") form short range unstructured order clusters in the liquid metal. At temperatures that are insignificantly over the metal's melting temperature, driven by van der Waals interaction, short range order clusters form cluster associates. It must be noted that the assumption that atoms form clusters with short range unstructured order does not contradict the experimental data that are indicative of non-crystalline nature of the short range order in liquid metals [30].

According to the model, the structure of the liquid metal undergoes a significant change in heating conditions if the degree of cluster association is (a) $a < 1$. Such a change is caused by individual clusters starting to destruct at $a < 1$, which leads to an increase in the number of atoms with "quasigas" dynamics.

According to the model, the dependence between the degree of cluster association a and temperature T is described by expression (1)

$$a(T) = a_2(T_2/T)^b, \tag{1}$$

where a_2 – the degree of cluster association at temperature T_2 derived from expression (2)

$$a_2 = \frac{\ln(\nu_2/\nu_1)}{\ln(T_1/T_2)}, \tag{2}$$

where ν_1 and ν_2 – the values of kinematic viscosity at temperatures T_1 and T_2. To calculate the temperature dependence $a(T)$, dynamic viscosity values $\eta(T)$ can be used.

Value b from expression (1) is the rate of decline of the degree of association of clusters in the temperature interval $T_2 \div T_3$. The value of b is calculated using expression (3)

$$b = \frac{\ln(a_3/a_2)}{\ln(T_2/T_3)}, \tag{3}$$

where a_3 – the degree of cluster association at temperature T_3 derived from expression (4)

$$a_3 = \frac{\ln(\nu_3/\nu_1)}{\ln(T_1/T_3)}, \tag{4}$$

Thus, to calculate dependence $a(T)$, we need to find the viscosity values at three reference space points and at pre-defined temperatures. It makes sense to choose the first reference point (ν_1, T_1) at a temperature that is somewhat above the metal's melting temperature; this way the influence of the crystalline phase on the viscosity should be ruled out. It makes sense to choose reference points (ν_2, T_2) and (ν_3, T_3) in the middle and in the end of the experimental array (ν_i, T_i) to ensure the maximum objectivity of the data obtained. It must be noted that the value of viscosity $\nu(T)$ of the liquid metal largely depends on the content of impurities and the method of measurement [31]. Because of this, the values of viscosity of liquid metals obtained by different authors may significantly differ.

3. Results and discussion

According to the cluster associate model of liquid metals structure, the destruction of short range order clusters takes place when the liquid metal reaches a temperature at which a sufficient amount of atoms exceeds the boiling point threshold. When a sufficient amount of atoms overcomes the boiling point threshold, local areas with quasigas atom dynamics are formed thus promoting local increases in the electric resistance and Joule heating. A local increase in Joule heating further increases the electric resistance which leads to the development of overheating instability.

To check this hypothesis we derived dependence T (a) to determine the temperature at which cluster destruction starts ($a = 1$). Dependence $T(a)$ was derived from equation (1) and written down as expression (5)

$$T(a)_{clust.destr.} = \frac{T_2}{\left(\frac{a}{a_2}\right)^{\frac{1}{b}}}\,a=1, \tag{5}$$

The values of coefficients a_2 and b were calculated using expressions (2)–(4). The temperature at which individual clusters are destructed in the liquid metal ($T_{clust.\ destr.}$) was determined from expression (5). The following metals have been selected for the calculations: Cu, Ni, Zn, Pb, Ag and Al. The calculation results are shown in Table 1. The values of the viscosity of liquid metals at respective temperatures were taken from works specified in the references in Table 1.

The analysis of the $T_{clust.\ destr}$ values obtained shows that they either do not exceed boiling temperature values for the respective metals or they are close to those. The data obtained are in accordance with the data in Ref. [9]. The authors have demonstrated that