Calculation of heat regimes for a Cr-Cu surface alloy formed with a low-energy high-current electron beam

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Abstract. The heat regimes for a Cr-Cu surface alloy formed on Cu substrate using liquid-phase mixing of film (Cr)-substrate (Cu) system with a low-energy, high-current electron beam (LEHCEB) have been studied. The calculations allowed to determine the melting thresholds for Cr and Cu and the optimal parameters of LEHCEB for Cr-Cu surface alloy formation. The calculations demonstrated that the melt thickness on the surface after irradiation with LEHCEB in optimal modes is 3-4 \( \mu \)m, and the lifetime \( \sim 1 \) \( \mu \)s. Mechanism of defect generation in the Cr particles was suggested. Generation is attributed to the action of tensile stresses owing to a large difference between the thermal expansion coefficients of Cr and Cu.

1. Introduction
A Cr-Cu alloy is a basic material for producing electrodes for high-current vacuum interrupters operating at medium voltages. A common method used for producing of Cr-Cu alloys is the powder metallurgy including powder sintering. The quality of electrodes manufactured by this method, however, has several drawbacks, the major ones are pores and oxygen present in the material [1]. The quantity of oxygen in material maybe so much that under certain conditions, sintering of the copper powder is followed by swelling of the components rather than their compaction, which is due to oxygen being intensively released in closed pores [1]. That is why the new methods of producing of Cr-Cu alloy are developing and one of them is method of formation of surface alloy with a low-energy, high-current electron beam (LEHCEB) [2]. Procedure of the method includes thin Cr film deposition on Cu substrate followed by surface melting of film (Cr)-substrate (Cu) system with a LEHCEB. The knowledge of heat regimes acting in the film-substrate system during irradiation is very important from the viewpoint of formation of surface alloy of good quality. This work deals with calculations of heat regimes in the film-substrate system at various parameters of LEHCEB. One more problem considered in the work deals with defects appearing in the layer of formed surface alloy.

2. Experimental
In order to calculate the temperature field in the film/substrate system, a 1D heat conductivity equation was solved, with the respective boundary and initial conditions. The melting process was simulated by the method of effective heat capacity, and the evaporation process was taken into consideration by the model of thermal damage [3]. In simulating the heat sources function, determining the energy released per unit volume of the target per unit of time, we used real waveforms of the cathode current and LEHCEB accelerating voltage. The temperature fields were calculated for different LEHCEB energy densities; the pulse duration \( \tau \) was 2.5 \( \mu \)s. Table 1 presents the thermal properties for chromium and
copper used in the temperature-field calculations in the system under study. The temperature
dependence of the thermal-physical material properties was taken from the reference books.

Table 1. Thermal properties of Cu and Cr.

| Material | $\rho$, kg/m$^3$ | $c$, J/(kgK) (at 300 K) | $k$, W/(mK) (at 300 K) | $T_m$, K | $q_m$, kJ/kg |
|----------|-----------------|-------------------------|------------------------|----------|--------------|
| Cu       | 8960            | 385.86                  | 201                    | 1356     | 204.6        |
| Cr       | 7200            | 444                     | 94                     | 2133     | 313.5        |

3. Results and discussion

Figure 1 presents the calculated melting thresholds of the film (1) and substrate (2) of the
Cr (film)-Cu (substrate) system as a function of the film thickness. The dashed lines show the melting
thresholds of pure Cu and Cr. It is evident that the melting threshold of the Cu substrate was found to
be 3.8 J/cm$^2$. In the course of the film deposition the melting threshold of the Cu substrate increases
practically in a direct proportion to its thickness and at the film thicknesses 1 and 4 $\mu$m it is equal to
4.3 and 6.7 J/cm$^2$, respectively. With unlimited increase in a film thickness, the melting threshold
tends to infinity.

The melting threshold for pure Cr is equal to 4.5 J/cm$^2$, while that of the system of a thin Cr film on
a Cu substrate is nearly a factor of 1.4 higher and is found to be 6.2 J/cm$^2$; this is associated with the
high heat conductance of Cu, which effectively removes heat from the Cr film and retards its melting.
The melting threshold of the Cr/Cu system does not change until the film thickness becomes 0.6 $\mu$m; it
is for thicker Cr films only that the film heat conductance begins strongly affecting the heat transfer
process and then gradually decreases, tending in the limit to the melting threshold of pure Cr.

As experimental investigations show the effective mixing of the film and substrate materials takes
place in the case of small thicknesses (usually of order~0.1 $\mu$m) of the deposited films. That is why
further simulations of the temperature fields were performed for the following system:
Cr film (0.1 $\mu$m)-Cu substrate (Cr(0.1)/Cu).

Figure 2 presents the dependence of the melted layer thickness on the LEHCEB energy density for
the Cr(0.1)/Cu system. A comparison of figures 1 and 2 demonstrates that the first melt portions
appear in the subsurface regions at the electron beam energy density $E \geq 3.8$ J/cm$^2$, with the substrate
only beginning to melt. As the energy density increases, the melt thickness on the surface of the target
increases nearly in a direct proportion. Starting at the energy density 6.2 J/cm$^2$, the film begins to melt
and soon the entire system is found in a liquid phase. It is clear that for effective melting of entire film-
substrate system the LEHCEB energy density should be more than 6.2 J/cm$^2$ (to the right of the red
circle in figure 2). The material evaporation is appearing at the LEHCEB energy density more than 7.0 J/cm². The latter is proved by deviation of the relationship from direct proportion. The larger is deviation the higher is energy loss for evaporation. In such a way, the optimal LEHCEB energy density for formation of Cr-Cu surface alloy is ranging from 6.3 to 7.0 J/cm².

![Figure 2. Dependence of the melted layer thickness on the LEHCEB energy density for the Cr(0.1)/Cu system.](image)

The temporal dependences of the melt thickness at the energy densities corresponding to the borders of optimal LEHCEB range 6.3 and 7 J/cm² are presented in figure 3. It is evident in figure 3a that an irradiation of the system under study by a LEHCEB at the minimal optimal energy density of 6.3 J/cm², the maximum melt thickness is 3.2 μm. The melting dynamics is the following: first, a layer of Cu below the Cr film surface begins to melt and in 0.43 μs the film itself melts. A common melt of Cr and Cu persists for ~0.2 μs, following which the film crystallizes on the surface of the target, and the copper substrate crystallizes as well. The average rate of the melt crystallization is 15.5 m/s. Under irradiation with LEHCEB at the energy density 7 J/cm², the maximum melt thickness is 4.3 μm (figure 3b). In this case the film melts in 0.26 μs after the onset of the substrate melting, and a common melt persists for ~0.94 μs, following which the film crystallizes on the surface of the target, and then the copper substrate crystallizes as well. The average rate of the melt crystallization is about 15 m/s.

![Figure 3. Temporal dependence of the melt thickness for the cases of irradiation of the Cr(0.1)/Cu system with LEHCEBs at the energy densities 6.3 (a) and 7 (b) J/cm².](image)

The results of calculations above reported imply that the Cu substrate only melts at the LEHCEB energy densities less than 6.2 J/cm², while the Cr film remains in a solid state. On the other hand, from
experiments it is evident that the concentration of copper on the surface irradiated in the regimes of 4.6 and 5.7 J/cm² energy density increases, which suggests that mixing of Cr and Cu does occur [4]. This result can be accounted for by the fact that in the calculations we used an average value of the LEHCEB energy density, while in the experiments it varies from shot to shot. These variations can be quite large, which undoubtedly affects the surface layer temperature regime as well. Earlier it was demonstrated numerically that a LEHCEB energy density scatter can result in considerable variations (several times) of the melted layer thickness [5]. Since in the experiments the number of pulses in each experimental series usually was equal to 10 or more, we might assume single shots to have been generated with the energy density higher than 6.2 J/cm², in which case not only the substrate but also the film might have melted. Thus, mutual mixing of the elements is also possible in the cases where the average LEHCEB energy density is lower than the melting threshold, provided the treatment is performed by a series of shots rather than in a single-shot mode.

In experimental work carried out, after irradiation of a Cr-Cu alloy specimen manufactured by the PM process, craters and cracks were observed on its surface [6, 7]. All cracks were found in Cr grains, while the craters were predominantly located either at the Cr grain junctions or even at the cracks. Authors report that in the Cu-25Cr and Cu-50Cr they did not observe any second-phase inclusions in either copper or chromium and that craters formed on the vacancy clusters or voids rather than on Cu and Cr inclusions, as it was demonstrated in steel or titanium alloys [8]. The formation of cracks was attributed to quasi-static pressures and low plasticity of Cr.

On our opinion in this case it is reasonable to refer to these defects as pores rather than craters, since there are no features of a classical crater, such as large transverse dimensions measuring tens or even hundreds of microns and a characteristic axis-symmetrical shape with a microhole in the center. On our opinion the mechanism of cracks formation in Cr grains is as follows. During crystallization of the surface melt, Cr particles are the first to crystallize, since the recrystallization temperature of Cr is nearly 800 K higher than that of Cu. Copper is the second to crystallize, and then the Cu-matrix and the Cr particles together undergo fast cooling. It should be recalled that Cr is a metal with a low thermal expansion coefficient, while that of Cu is by 2-3 factors higher. Thus during cooling a particle of Cr would be affected by tensile stresses from the copper matrix. The value of these stresses can be estimated using the formula

$$\sigma = E\Delta\alpha\Delta T,$$

where $E$ is the Young modulus, $\Delta\alpha$ is the difference between thermal expansion coefficients of Cr and Cu, and $\Delta T$ is the difference between the crystallization and room temperatures.

The estimations performed by this formula yield $\sigma=2–3$ GPa, which is a few times higher than the ultimate tensile strength of chromium. Thus, it is evident that it is the tensile stresses operating during cooling which cause cracking.

4. Conclusions

The heat regimes for a Cr-Cu surface alloy formed on Cu substrate using liquid-phase mixing of film (Cr)-substrate (Cu) system with a low-energy, high-current electron beam (LEHCEB) have been investigated. The calculations allowed finding of melting thresholds for Cr and Cu and statement of the optimal parameters of LEHCEB for Cr-Cu surface alloy formation. The optimal energy density in the range from 6.3 to 7 J/cm² has been found for Cr-Cu surface alloy formation. The calculations demonstrate that the melt thickness on the surface after irradiation with LEHCEB in optimal modes is 3-4 μm, and its lifetime ~1 μs.

Generation of cracks in Cr particles is attributed to the action of tensile stresses owing to a large difference between the thermal expansion coefficients of Cr and Cu. During cooling a particle of Cr would be affected by tensile stresses from the Cu matrix. The value of these stresses is 2-3 GPa, which is a few times higher than the ultimate tensile strength of Cr.
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References
[1] Papillon A, Roure S, Schellekens H, Missiaen J M, Chaix J M and Rigal E 2017 Mater. Des. 113 353
[2] Markov A B, Mikov A V, Ozur G E and Padei A G 2011 Instrum. and Experim. Tech. 54 862
[3] Rotshtein V, Ivanov Y and Markov A 2006 Surface Treatment of Materials with Low-Energy, High-Current Electron Beams, in: Mater. Surf. Process. by Dir. Energy Tech. (Elsevier) 205
[4] Report to RFBR Research Project N 16-08-00920A, 2017
[5] Markov A B and Rotshtein V P2000 High Temp. 38 15
[6] Zhou Z M, Chai L J, Xiao Z P, Tu J, Wang Y P and Huang W J 2015 Trans. Nonferrous Met. Soc. China 1935
[7] Chai L J, Zhou Z M, Xiao Z P, Tu J, Wang Y P and Huang W J 2015 Sci. China Technol. Sci. 58 462
[8] Zou J, Zhang K, Dong C, Qin Y, Hao S and Grosdidier T 2006 Appl. Phys. Lett. 89