Calculation of heat regimes for a Ni-Al surface alloy formed on a carbon steel substrate with a low-energy high-current electron beam

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Abstract. In the present work, the calculations of heat regimes for a Ni-Al surface alloy formed on a carbon steel substrate using a low-energy high-current electron beam (LEHCEB) were carried out for two types of multilayered systems with different numbers and thicknesses of the layers. The multilayered system of type 1 was a three layered system Ni (0.5 µm)-Al (1.52 µm)-Ni (0.5 µm). The multilayered system of type 2 consists of 10 layers of Ni (0.1 µm each) alternating with 9 layers of Al (0.167 µm each). The total thickness of coating deposited in both cases was 2.5 µm. The melting thresholds for Ni, Al and carbon steel during LEHCEB irradiation were determined by the calculation. The phase diagrams obtained in calculation showed that process of melting occurs similarly for both types of multilayered systems. The calculation demonstrated that the melt thickness on the surface after irradiation by LEHCEB with optimal parameters is about 3 µm, and the average lifetime of the melt is ~ 1 µs (Ni-layers), and ~ 10 µs (Al-layers).

1. Introduction
Heat resistant alloys based on nickel-aluminum are widely used nowadays in engineering technologies, for example, for the aircraft industry. They have high thermal conductivity combined with high strength at elevated temperatures. Abovementioned properties as well as its low density make NiAl alloy ideal for special applications like coating blades in gas turbines and jet engines [1, 2]. Moreover, NiAl alloy possesses the high module of elasticity and high corrosion resistance, which gives an opportunity to use it like corrosion resistance coating.

To form the Ni-Al surface alloy on carbon steel the films of Ni and Al are deposited alternatively on a substrate of carbon steel (0.14–0.22% C; 0.15–0.3% Si; 0.4–0.65% Mn, 0.3%Ni; 0.3% Cr; Fe – balance, wt.%). Then this multilayer system is exposed to action of a low-energy, high-current electron beam (LEHCEB) which induces a liquid-phase mixing of deposited elements. The purpose of the work and, consequently, the calculations carried out was to determine optimal parameters of a LEHCEB for Ni-Al surface alloy formation on carbon steel and to investigate the effect of different thicknesses of layers of Ni and Al on the heat regime of a target. The latter is important because in terms of liquid-phase mixing the thin layers are more preferable but for simplification and cheapening of technological process the thicker layers are better.
2. Modeling and results

The calculations were carried out for two types of multilayered systems with different thickness and numbers of the layers. The multilayered system of type 1 was a three layered system Ni (0.5 µm)-Al (1.52 µm)-Ni (0.5 µm). The multilayered system of type 2 consists of 10 layers of Ni (0.1 µm each) alternating with 9 layers of Al (0.167 µm each). The substrate was carbon steel. The total thickness of Ni-layers and Al-layers was 2.5 µm for both types of multilayered systems.

Thermal calculations were carried out according to the procedure described elsewhere [3]. Values of thermal properties of materials used in calculations are given in table 1 [4]. Here $\rho$, $c$, $k$, $T_m$, and $L_m$ are density, heat capacity, heat conductivity, melting point, and latent heat of melting, respectively. Calculations were carried out for a single pulse with an electron energy of 25 keV and duration of 2.6 μs.

| Material   | $\rho$ (kg·m$^{-3}$) | $c$ (J·kg$^{-1}$·K$^{-1}$) at 300 K | $k$ (W·m$^{-1}$·K$^{-1}$) at 300 K | $T_m$ (K) | $L_m$ (kJ·kg$^{-1}$) |
|------------|----------------------|-----------------------------------|----------------------------------|-----------|----------------------|
| Al         | 2700                 | 902.5                             | 237                              | 933.3     | 396.6                |
| Ni         | 8600                 | 439                               | 64                               | 1726      | 303.2                |
| Carbon steel | 7850            | 460                               | 56                               | 1600      | 205                  |

As a result of calculations it was obtained that melting thresholds of pure Al, Ni and carbon steel are 2.4, 3.8 and 2.1 J·cm$^{-2}$, respectively. The melting threshold for a multilayer system of type 1 was 4.3 J·cm$^{-2}$ and for multilayer system of type 2 was 4.4 J·cm$^{-2}$. Figure 1 shows the dependence of the thickness of the melted layer formed on the irradiated surface on LEHCEB energy density. The first portion of melt, in case of type 1 multilayer system, appears at energy density of LEHCEB 1.6 J·cm$^{-2}$, in a layer of aluminum, i.e. beneath the irradiated surface. As energy density increases, the thickness of the aluminum layer melt rise. At energy density equals to 1.9 J·cm$^{-2}$, Al layer is melting completely. Further, the thickness of the melt does not change with the increase in the energy density, the lifetime of the melt grows only. At 3.5 J·cm$^{-2}$, the Ni-layer located on the irradiated surface begins to melt, then the melt appears in the substrate material, and finally in the Ni-layer lying close to the substrate. At melting threshold energy density (4.3 J·cm$^{-2}$), all the layers and partially the substrate material have melted. The melting threshold is depicted on the curve by a larger dot. With further increase in energy density, the thickness of the molten layer continues to grow almost linearly. At energy densities of more than 7 J·cm$^{-2}$, the dependence diverges from linear, because more and more energy is spent on evaporation of the material from the irradiated surface.

![Figure 1](image-url)  
**Figure 1.** The dependence of thickness of the melted layer on LEHCEB energy density. Curves 1 and 2 corresponds to type 1 and 2 multilayered system, respectively. The larger symbols on curves 1, 2 depict energy densities corresponding to melting thresholds for multilayered systems.

As can be seen from the picture, the dependence of the molten layer thickness on the energy density for a type 2 multilayer system is very close to one for a type 1 multilayer system. It is visible
the appearance of the melt at the energy density of 1.6 J cm⁻². Melting begins in Al-layer closest to the irradiated surface. All Al-layers are melted one by one with the rise of energy density. The nickel layers begin to melt later. Melting in the substrate material begins before melting of the Ni layer lying on the substrate. The significant different between curves 1 and 2 is in the range of energy density from 2 to 4 J cm⁻². This difference is explained by the different geometries of these multilayer systems, namely, the number and thickness of Ni- and Al-layers. Dynamics of the melting of both multilayer systems is very similar.

Figures 2 and 3 show the state diagrams of the type 1 and type 2 multilayer systems during LEHCEB irradiation with energy densities corresponding to the melting thresholds of these systems, respectively. Depending on the state of the material, the areas on the diagrams are painted dark grey (liquid phase), light grey (so-called slush or two-phase state), and white (solid phase). As for two-phase or slush state this term means the state of the material in which it is heated to its melting point but not yet completely melted, since the released latent heat is below the latent heat of the melting.

Figure 2. A diagram of the state of a type 1 multilayer system under irradiation by LEHCEB with an energy density of 4.3 J cm⁻².

Figure 3. A diagram of the state of a type 2 multilayer system under irradiation by LEHCEB with an energy density of 4.4 J cm⁻².

Diagrams of the state show that regardless of number of layers in the system, Al-layers are the first to melt. The Al-layers are melting rapidly, one by one, starting from the layer closest to the irradiated surface. Calculations have shown that in both multilayer systems the first portion of the melt appears in about 0.6 µs after the beginning of irradiation, in the aluminium layer closest to the irradiated surface. For a type 1 multilayer system, about 0.3 µs is required to melt the Al-layer completely. For a type 2 multilayer system, thinner Al-layers have melted completely one by one in 0.2 µs. The melting of Ni-layer on the irradiated surface in a type 1 multilayer system occurs in 0.2 µs after Al layers melting, and further the melting of the substrate material begins. The thickness of the molten layer in the substrate reaches about 0.6 µm. Melting of nickel layer lying on substrate takes place in 0.4 µs. In a multi-layer type 2 system, the melting of one nickel layer takes from 0.06 to 0.11 µs. The melting of the material of the substrate also begins earlier the all Ni-layers are melted. For melting of all layers of a type 1 multilayer system it takes a little bit more than 1.6 µs. All layers of the type 2 multilayer system are melted in 1.8 µs. The maximal value of melt thickness from the surface was 3.1 µm for both multilayered systems. As it can be seen from the diagrams, the crystallization process in both multilayered systems begins in Ni-layer lying on the substrate. Crystallization of Ni-layers takes approximately 0.2 µs. Then the Al-layers crystallize.
3. Conclusion
By simulating of temperature fields in type 1 and 2 multilayer systems, optimal LEHCEB parameters for Ni-Al surface alloy formation on carbon steel were determined. It is obtained that the optimum energy density for type 1 and 2 multilayer systems is 4.3 and 4.4 J cm\(^{-2}\), respectively.

No significant influence of the number and thickness of layers on thermal conditions was found in the considered multilayer systems.

References
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