Heat distribution simulation in electron-beam surface modification of 316L stainless steel samples

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Abstract. A time-dependent heat model is implemented for the simulation of the heat distribution in 316L stainless steel samples during electron-beam irradiation. The influence is studied of the electron-beam power and processing time on the temperature field produced in the samples. The simulation results are compared with real experimental data of electron-beam surface modification of 0.5-mm-thick 316L stainless steel samples using the ELIT-60 installation in the Institute of Electronics BAS. The simulation and the experimental results show good agreement.

1. Introduction
Due to its excellent properties and very good weldability, the austenitic 316/316L stainless steel has numerous applications in the production of food-processing equipment; brewery, dairy and pharmaceutical production equipment; chemical and petrochemical equipment; laboratory benches and equipment; coastal architectural paneling; chemical transportation containers; heat exchangers; pulp and paper equipment; film-processing equipment; pipelines; equipment for marine, food and fertilizer production industries and many others.

A large amount of research results have been reported concerning software products and applications for simulation of the temperature distributions with various heat sources [1-7] (electron beam, laser [4], plasma arc, etc.) and different materials and processes (melting [5], additive manufacturing [3,7], welding [1,6], micro-welding, casting, cutting, surface modification, etc.). In our previous studies, we have developed quasi-steady state and time-dependent thermal models and applied them to the simulation of the processes of electron-beam melting and refining and electron-beam welding of different materials [5, 8-14]. They have been based on different assumptions for the type of the heat source – point, linear, exponential, combined, etc. The solutions of the thermal physical models yield approximations of the shape of the temperature distributions, taking into

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account the parameters of the processes and materials. The assumptions adopted in the physical models make it difficult to evaluate precisely the experimental results. These models are being developed to estimate the temperature distributions and the shapes of the melted and heat-affected zones in view of optimizing the process parameter aiming to produce the required geometry, structure, level of refining, etc. Our earlier studies on electron-beam surface modification of reactive metals and 316L stainless steel (SS) samples by electron-beam surface melting and/or heating have been presented in [15, 16]. In [17], the local mechanical properties of welded 316H SS pipes were investigated by implementing a digital image correlation method by strain mapping. The effect of the heating conditions on the strength, hardness and microstructure of the 316L SS was studied in [18]. Papers [19, 20] presented the changes in the microstructures and the mechanical properties for different cases of electron-beam welding. In [21], the effects of radiation on deformation of metallic materials were reviewed.

In [16], the surface of samples of austenitic stainless steel 316L was modified in the ELIT-60 electron-beam installation in IE BAS using different electron-beam powers and different irradiation duration times in order to investigate the changes in their mechanical properties: 0.2% proof strength $R_{0.2}$, tensile strength $R_m$ and percentage elongation after fracture $A_{50}$. The thickness of the irradiated samples was 0.5 mm; figure 1 illustrates their dimensions and the area irradiated by the defocused electron beam.

![Figure 1. Dimensions of the irradiated samples (mm) and the area irradiated by the electron beam.](image)

During the experiments, the vacuum in the chamber of the electron-beam installation was $10^{-2}$ Pa, the focal length was 340 mm and the spot size with a diameter of 20 mm was changed to 25 mm by changing the deflection angle. During some of the experiments, the surface temperature reached the melting temperature of 316L SS. We avoided the formation of a molten pool in order to prevent the changes in the samples’ crystal structure.

Usually, the mechanical properties (besides the geometry of the molten pool) of electron-beam-welded samples are studied by tensile tests to investigate the connection with the variation of the process parameters [17, 19-20]. The study presented here deals with regimes of electron-beam exposure that heat the 316L SS samples up to temperatures lower than their melting temperature. Such temperatures are observed, for example, during electron-beam welding in areas adjacent to the molten pools. The parameters of sample surface heating – electron-beam power and irradiation duration – have a combined effect on the mechanical properties of the treated samples [16]. To investigate the relation of the mechanical properties and the microstructures obtained with the process parameters, a combination of experimental, empirical and numerical modelling should be applied. The current paper aims to develop a time-dependent thermal model for the case of electron-beam surface modification considered, taking into account the specific heat treatment, the concrete geometry and the temperature-dependent 316L SS material characteristics. The first step in the development of such a model is to estimate the dependencies of the material characteristics – specific heat capacity, thermal conductivity density, thermal diffusivity, etc. – on the temperature in a wide thermal region (during welding the material can be overheated and the temperatures can reach some hundreds of degrees above the melting temperature). Second, the desired geometry of the irradiated samples should be provided in order to formulate the boundary conditions. The model should then be verified experimentally.

Estimating the adequacy of a time-dependent thermal model for electron-beam surface modification of 316L SS samples will help in understanding how the changes of the mechanical properties and in the microstructures of the treated 316L SS samples are connected with concrete temperature distributions (specifically, maximum temperatures, thermal gradients and cooling rates) and thus to a concrete process parameters combination.
2. Thermal model
We consider a three-dimensional time-dependent thermal model to analyze the heat flow and the resulting temperature distribution over the irradiated sample’s area. The thermal processes can be described by the differential heat-conduction equation:

\[ c_p(T) \rho(t) \frac{dT}{dt} = \frac{\partial}{\partial x} \left( \lambda(T) \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \lambda(T) \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( \lambda(T) \frac{\partial T}{\partial z} \right) \]  

(1)

The material characteristics, namely, the specific heat capacity \( c_p(T) \) [J/kg K], and the thermal conductivity \( \lambda(T) \) [W/m K] and density \( \rho(T) \) [kg/m^3] are temperature-dependent.

A set of appropriate boundary conditions takes into account the radiation losses and the heating-beam energy distribution with a correction accounting for the secondary electron energy losses [5]. There, three types of heat contact areas between the ingot and the crucible are assumed: (i) areas with an ideal heat contact described by the Fourier equation; (ii) areas with a Newton-type heat contact; and (iii) areas in which the radiation losses predominate. They are given according to the interfaces: \( G_1 \) – on the top of the sample (the irradiated area, figure 1), \( G_2 \) – on the top of the sample (the area not irradiated) and the sidewalls of the sample, and \( G_3 \) – on the bottom of the sample (contact area with a large stainless steel block on which all processed samples are placed during irradiation in the vacuum chamber). Denoting the energy distribution by \( \tilde{g} = (x, y, z, t) \), the corresponding boundary conditions are:

\[ \lambda_1(T) \times \frac{\partial T}{\partial z} (\tilde{g}) = -P_n(x, y) + \varepsilon(T) \times \sigma \times \left( T^4(\tilde{g}) - T_{st}^4 \right) \]  

(2)

\[ \lambda_1(T) \times \frac{\partial T}{\partial x} (\tilde{g}) = -\varepsilon(T) \times \sigma \times \left( T^4(\tilde{g}) - T_{st}^4 \right) \]  

(3)

\[ \lambda_1(T) \times \frac{\partial T}{\partial z} (\tilde{g}) = \lambda_2 \times \frac{\partial T}{\partial z} (\tilde{g}) \]  

(4)

where \( \varepsilon \) is emissivity, \( \sigma \) is the Stefan-Boltzmann constant \((5.67 \times 10^{-8} \text{ W/(m}^2 \text{ K}^4))\), \( \lambda \) is the thermal conductivity, \( T_{st} \) is the ingot surface temperature. The heat transfer coefficient on the boundary area \( G_3 \) is assumed \( \lambda_1/\lambda_{3st} = 0.8 \). The energy transfer coefficient for electron-beam irradiation is considered 90%. This reduction of the effective energy input is due mainly to losses by backscattered electrons. The heat source is assumed to have a Gaussian distribution for an electron beam with a 10-mm radius. In the case considered here, losses arise also due to irradiation of areas around the sample (figure 1). The effectively irradiated area of the sample is calculated as 32% of the area totally covered by the electron beam. Table 1 presents the models for the temperature-dependent material characteristics, estimated and used for the calculations for 316L SS and based mainly on the recommended data for SS 316 in [22]. They are verified by the data available in [23-26] for stainless steel 316L.

The initial condition of a uniform temperature distribution at time \( t = 0 \) can be set as:

\[ T(x, y, z, t)|_{t=0} = T_0, \]  

(5)

where \( T_0 \) is the ambient temperature of 298 K (25 °C). The melting temperature of 316L steel is \( T_m = 1673 \text{ K} \) [13] (\( T_s = 1633 \text{ K}, T_l = 1683 \text{ K} \)). Mechanically-polished surfaces of steel 316 [22] in high vacuum have a normal emissivity \( \varepsilon \) values of 0.1 to 0.2.

In the mushy region (for temperatures between \( T_s \) and \( T_l \), the values of the temperature-dependent properties \( P_T \) (like specific heat capacity, density, thermal conductivity, emissivity, etc.) can be calculated by [22]:

\[ P_T = f_{s(T)} P_{Tsol} + (1 - f_{s(T)}) P_{Tliq}, \]  

(6)

where \( f_{s(T)} \) is the fraction of the solid material at temperature \( T \) and \( P_{Tsol} \) and \( P_{Tliq} \) are values of the property at the solidus and at the liquidus temperatures. The approximation in table 1 for the mushy zone is done by linear models defined by the material characteristics’ values estimated at \( T_{sol} \) and \( T_{liq} \).
Table 1. Temperature-dependent material characteristics of SS 316.

| Parameter                          | Model                                                                 | Temperature range, K |
|------------------------------------|----------------------------------------------------------------------|----------------------|
| Specific heat capacity, J/(g K)    | $C_{pS} = 0.449324477 + 0.000166157T - 2551.42527T^2$                 | 298–1633             |
|                                    | $C_{pSL} = -2.873 + 0.00227T$                                        | 1633–1683            |
|                                    | $C_{pL} = 0.83$                                                      | $T \geq 1683$        |
| Thermal conductivity, W/(m K)      | $\lambda_S = 4.227 + 0.03602T - 1.795 \times 10^{-5}T^2 + 3.806 \times 10^{-9}T^3$ | 298–1633             |
|                                    | $\lambda_{SL} = 169.9 - 0.08459T$                                   | 1633–1683            |
|                                    | $\lambda_L = -209.6 + 0.25317T - 6.667 \times 10^{-5}T^2$            | 1683–1873            |
|                                    | $\rho_S = 811.3 - 0.5074T$                                          | 298–1633             |
| Density, g/cm$^3$                  | $\rho_{SL} = 19469.846 - 7.462T$                                    | 1633–1683            |
|                                    | $\rho_L = 8200 - 0.7657T$                                           | $T \geq 1683$        |
| Thermal diffusivity, $10^6$ m$^2$/s| $a_S = 1.94 + 0.006648T - 3.667 \times 10^{-4}T^2 + 6.865 \times 10^{-10}T^3$ | 298–1633             |
|                                    | $a_{SL} = 45.54 - 0.02421T$                                         | 1633–1683            |
|                                    | $a_L = -42.62 + 0.05061T - 1.333 \times 10^{-5}T^2$                  | $T \geq 1683$        |
| Total normal emissivity            | $\varepsilon_N^* = 0.0627 + 0.0001T$                                | 298–1633             |
| Total hemispherical emissivity     | $\varepsilon_T = 0.1475 + 0.0002488T - 5.5 \times 10^{-8}T^2$       | 298–1025             |

$^*$ (highly polished in vacuum); $^{**}$ (extrapolated)

3. Experimental and simulation results

The experiments [10] were performed by irradiating 0.5-mm-thick 316L stainless steel samples (figure 1) in the vacuum electron-beam installation at different values of the process parameters – the electron-beam power was varied at three steps: 0.6 kW, 0.75 kW, and 0.9 kW and different irradiation times were applied (from 1 s to 120 s). The structure of a not irradiated sample is presented in figure 2. The examination of the metallographic structure showed that in the initial material (not treated sample) the structure is single-phase-austenitic. The microscope magnification is ×500.

Figure 3 and figure 4 present the microstructures of 316L stainless steel samples irradiated at two electron-beam powers: 0.6 kW and 0.75 kW for 90 s. The analyses of the test specimens show that at different electron-beam powers and at different exposure times, the structures produced are different. A layered structure is mainly observed as a result of surface layer-melting by the electron beam. The non-equilibrium crystallization conditions determine the differences in the crystal formation. The formed colonies of large and small dendrites are disoriented with respect to each other. The structural modification observed is connected with changes in the mechanical properties [16] of the irradiated samples.

Figure 2. Microstructure of non-irradiated 316L SS sample (×500 magnification).

Figure 3. Microstructure of 316L SS sample irradiated at electron-beam power of 0.6 kW for 90 s (×500 magnification).

Figure 4. Microstructure of 316L SS sample irradiated at electron-beam power of 0.75 kW for 90 s (×500 magnification).
In order to determine the temperature distributions caused by the electron-beam surface treatment and leading to changes in the structure and the mechanical properties of the samples, we applied the three-dimensional time-dependent thermal model described [5] at the appropriate boundary conditions.

Figure 5 and figure 6 show the calculated temperature fields for the irradiated 316L SS samples at different electron-beam powers and processing times. The corresponding maximal temperatures are 754.72 K and 1072.9 K.

![Figure 5. Temperature fields in the 316L SS sample irradiated at electron-beam power of 0.6 kW for 60 s.](image1)

![Figure 6. Temperature fields in the 316L SS sample irradiated at electron-beam power of 0.75 kW for 90 s.](image2)

4. Conclusions
Electron-beam irradiation is used to modify the surface of 0.5-mm-thick stainless steel 316L samples. A time-dependent thermal model is developed for the case considered of electron-beam surface modification taking into account the specific heat treatment, the concrete geometry and the temperature-dependent material characteristics. The dependencies are estimated of the specific heat capacity, the thermal conductivity density, the thermal diffusivity, etc. on the temperature in a wide thermal region. The desired geometry of the irradiated samples is provided in order to take into account the boundary conditions.

The estimation of an adequate time-dependent heat model for electron-beam surface modification of 316L SS samples will assist in understanding how the changes of the mechanical properties and of the microstructure of the treated 316L SS samples are related to specific temperature distributions (particularly, maximum temperatures, thermal gradients and cooling rates) and thus to concrete combination of process parameters. Conclusions can be made on the choice of working regimes not only for electron-beam surface modification, but also for other processes, such as electron-beam welding of thin plates or electron-beam micro-welding.

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