Computer simulation of metals ionization process during electron-beam welding

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Abstract. One of the most actual problems during electron beam welding of metal materials is the determination of the laws of primary electrons interaction with a gas (vapor) flow, taking into account existing and generated (by charged particles) electric fields. The paper is devoted to the development of computer simulation method for the process of electron beam passage through a layer of evaporated metal. The analysis of simulation results showed a significant effect of ionization process on electric field in a gas-vapor channel. It was established that at the initial stage of the process, a region with a positive potential is formed in the lower part of gas-vapor channel, and in its upper part, on the contrary, potential decreases.

1. Introduction
Currently, many areas of machine-building production are intimately associated with making such products that are subject to increased requirements for strength, ductility, corrosion resistance, etc. One of the promising areas that can successfully overcome different technological difficulties arising during the process of such products making is electron beam processing. Electron beam heats metal (during electron deceleration), causes its melting and evaporation.

One of the most actual tasks is to determine the laws of interaction of primary electrons with a gas (vapor) flow, taking into account existing electric fields and generated by charged particles. Therefore, this paper is devoted to the development of computer simulation method for the process of electron beam passage through a layer of evaporated metal.

2. Method of computer simulation
As the initial data for modeling, it is necessary to set medium density or concentration of particles $\eta$. It is known [1] that density of particles above the surface of penetration channel is about $10^{17}$ per 1 cm$^3$, and above the surface of molten metal (at the bottom of the channel), it approaches to the density of particles in the solid state, i.e. it is about $10^{24}$ in 1 cm$^3$. The computer simulation process was performed for aluminum.

In addition to ionization, the process of electron passage through a vapour layer will be accompanied by energy losses for other types of interactions, for example, excitation of phonons, plasmons, deceleration radiation generation and recombination processes. In addition, it is possible to change the direction of primary electrons motion due to elastic interactions [2]. The purpose of this
study is to analyze ionization processes, potential distribution and ionization losses. In the simulation process, we shall consider inelastic interaction cross-section — ionization cross-section of gas (vapour) molecules by electron impact. As is known, ionization cross-section of an atom or molecule by electron impact is a function of electron energy [3]. Typically, ionization cross-section is about $10^{-16}$–$10^{-17}$ cm$^2$. The dependence of ionization cross-section of aluminum atom ($\sigma_{Al}$) on electron energy used in the proposed model is shown in Figure 1. The model diagram is shown in Figure 2. Target 1 (product) of aluminum has a cylindrical shape, its lateral and lower faces are grounded (the potential is taken equal to zero). The gas-vapor channel in the model is approximated by normal distribution function (item 2 in Figure 2). The distribution of vapors density spreading in vacuum 3 in the channel and beyond it is specified. Potential on the channel wall and on the upper surface of cylinder is determined by field potential created by electron beam 4. Electron flux density obeys the normal distribution function. Ionization processes occur in the vapor-gas channel, and charged particles move under the action of Lorentz forces in the field, created by the particles themselves. This field does the work and changes trajectories of the particles.

![Figure 1](image-url)

**Figure 1.** Dependence of ionization cross-section for aluminum atom on electron energy: $T_i$ – electron energy values, eV; $\sigma_i$ – values of ionization cross-section, × 10$^{16}$, cm$^2$ [7]

The calculation of electric field is carried out in an axially symmetric formulation. For this case, the equation can be used

$$\frac{\partial^2 U}{\partial r^2} + \frac{1}{r} \frac{\partial U}{\partial r} + \frac{\partial^2 U}{\partial z^2} = -\frac{\rho(r,z)}{\varepsilon_0},$$

where $U$ is electric potential (V); $r$ and $z$ are radial and axial coordinates, respectively (m), $\varepsilon_0$ is permittivity of vacuum (F∙m$^{-1}$); $\rho(r,z)$ is volume density of spatial charge created by charged particles beam in the zone of field action (C∙m$^{-3}$). Its equation can be written as

$$\rho = \frac{dQ}{dV},$$

where $dQ$ is charge part, distributed over the elementary volume $dV$. A cylindrical grid is superimposed on two-dimensional computational region, cells of which are numbered along $r$-axis as $i = 0,1,2 \ldots i_{\text{max}}$, and along $z$-axis as $j = 0,1,2 \ldots j_{\text{max}}$ (Figure 2). The sizes of cylindrical grid cells are $\Delta r$ and $\Delta z$, respectively. In accordance with selected grid scheme, calculation values $U_{i,j}$ are performed in consecutive order for all nodes of the grid and are stored in the data array $U(i,j)$. A finite-difference approximation of computational region was used, for which equation (1) can be written as

$$\frac{U_{i+1,j} - 2U_{i,j} + U_{i-1,j}}{\Delta r^2} + \frac{1}{i\Delta r} \frac{U_{i+1,j} - U_{i,j}}{\Delta r} + \frac{U_{i,j+1} - 2U_{i,j} + U_{i,j-1}}{\Delta z^2} = -\frac{\rho_{i,j}}{\varepsilon_0},$$

(3)
Figure 2. Diagram of two-dimensional model of the process of metal vapor ionization in a gas-vapor channel: 1 - grounded product; 2 - gas-vapor channel; 3 - vacuum, metal vapor; 4 - electron beam; 5 - equipotentials; elements of the computational grid and diagram of electron impact ionization process are shown on the right

This equation was solved by the method of Euler. Then, using grid function \( U(i,j) \) obtained, vector field of electric field strength \( \vec{E} \) (V/m) was calculated by numerical differentiation

\[ \vec{E} = -\text{grad}U, \quad (4) \]

as well as projections of this vector on the coordinate axes \( E_r \) and \( E_z \) for each node of the computational grid. The acceleration components, acquired by a particle when moving in an electrostatic axially symmetric field due to the Coulomb force, are determined from the equation

\[
\begin{aligned}
    a_r &= \frac{qE_r}{m}, \\
    a_z &= \frac{qE_z}{m} 
\end{aligned}
\]

where \( a_r \) and \( a_z \) are the radial and axial components of acceleration (m/s\(^2\)); \( q \) is particle charge (C); \( m \) is particle mass (kg). The task of particle trajectory calculating is solved with a fixed time integration step (which was taken equal to \( 10^{-12} \) s). Equations for the projections of speeds increments \( \Delta v_r, \Delta v_z \) and coordinates increments \( \Delta S_r, \Delta S_z \) of the particle in the time interval \( (\tau_1, \tau_2) \) are written as follows:

\[
\begin{aligned}
    \Delta v_r &= \frac{q}{m} \int_{\tau_1}^{\tau_2} E_r \, dt, \\
    \Delta S_r &= \int_{\tau_1}^{\tau_2} v_r \, dt, \\
    \Delta v_z &= \frac{q}{m} \int_{\tau_1}^{\tau_2} E_z \, dt, \\
    \Delta S_z &= \int_{\tau_1}^{\tau_2} v_z \, dt. 
\end{aligned}
\]

(6)

(7)

The distribution of current density in the product was calculated on the basis of Ohm's law in differential form

\[ j = \gamma E, \]

(8)
where \( j \) is current density vector (A\( \cdot \)m\(^{-2}\)), \( \gamma \) is specific conductivity of product’s material (aluminum), Ohm\(^{-1}\)\( \cdot \)m\(^{-1}\).

The most difficult stage of the problem to solve is simulation of ionization process, which is accompanied by energy exchange between particles and appearance of a free electron. In accordance with definition of the term “interaction cross-section” [4], mean free path of an electron \( \lambda_i \) between ionization acts is defined as

\[
\lambda_i = \frac{1}{\eta \sigma_i},
\]

where \( \eta \) is concentration of aluminum atoms (m\(^{-3}\)). Concentration of atoms is related to vapor pressure by ideal gas law

\[
\eta = \frac{P}{kT},
\]

where \( T \) is vapor temperature, \( k \) is Boltzmann constant. At the current stage of research, a linear approximation of pressure distribution function over the channel depth \( P(z) \) was used, which is agree with published works [5].

To take into account random nature of vapour particles distribution, the Monte Carlo method [6] was used. In this case, path \( s_i \), which electron passes between ionization acts, will be determined by the equation

\[
s_i = -\lambda_i \ln(1 - R_i),
\]

where \( R_i \) is a dimensionless random value, uniformly distributed in the range from 0 to 1. As a result of ionization, a pair of such particles, as positive ion and slow electron, appears; their trajectories will also need to be calculated in each time interval.

The initial energy of secondary electron \( W_s \) (eV), which appeared as a result of ionization, is proposed to determine by the equation

\[
W_s = \omega \cdot \tan \left( R_2 \arctan \left( \frac{W_p - J}{2\omega} \right) \right),
\]

where \( W_p \) is energy of bombarding (primary) electron (eV); \( J \) is ionization potential; \( \omega \) is tabular value, obtained by comparing theoretical and experimental data (for aluminum this value is equal 2.7 eV); \( R_2 \) is a dimensionless random value, uniformly distributed in the range from 0 to 1.

In the case considered above, primary electron energy loss due to ionization \( \Delta W_{pi} \) (eV), was calculated by the equation

\[
\Delta W_{pi} = J + W_s.
\]

Path that an electron travels between elastic interaction acts \( s_e \) is determined by the equation

\[
s_e = -\lambda_e \ln(1 - R_3),
\]

where \( R_3 \) is a dimensionless random value, uniformly distributed in the range from 0 to 1.

In order to study ionization processes, calculations in accordance with expressions (1)–(14) were implemented in the Elion program module in C++.

3. Results of simulation and their discussion

At the current stage of research, the most interesting was information on the distribution of electric field potential, created by particles in the penetration channel and near it, as well as spatial distribution of particle ionization density acts. Figure 3 shows the results of computational experiments, realized on a personal computer with an IntelCorei7-6700 HQ processor.

Figure 3a shows the case corresponding to the absence of aluminum vapor concentration (it is equal to zero) in the region above penetration channel. This situation corresponds to the initial stage of electron beam impact on the target (in the real case, penetration channel is not formed yet, and sample
surface is flat). The beam current is 18 mA. It is seen that a region with the smallest electric potential is in the beam center. In the approach to the bottom of the channel, potential increases, approaching almost to zero, since potential difference between the channel bottom surface and the lowest (grounded) plane of the product is negligible for this case. The minimum potential value under electron beam steady action on the product without taking into account beam interaction with metal vapors is equal to $-1.8 \text{ V}$. In the case when vapor pressure distribution of aluminum along $Z$-axis is specified, the picture changes radically: potential distribution will be completely different after a time on the order of 0.05 ns. Figure 3b shows such a case. Vapor pressure of aluminum in the lowest part of the channel is 30 Pa, and at the point $z = 0$ (at the distance of 2 mm above the product surface) it is equal to 0.1 Pa. The dependence $P(z)$ at this stage of the research was assumed to be linear.

![Electric field distribution](image)

**Figure 3.** Electric field distribution: a) in the channel in the absence of metal vapor, b) taking into account linear distribution of vapor pressure along coordinate $z$. 
Ionization of neutral aluminum atoms leads to the appearance of positively charged ions and slow electrons. Due to the fact that electron beam has a current density distribution over its radius, most of ions appear precisely in the center of the beam, and at the initial stage of ionization process, shown in Figure 3,b, slow electrons will also appear near the center of the beam. Under the action of positive ions field, localized mainly in the center of the beam, peripheral slow electrons will drift in their direction, creating a sharp minimum of potential in the center.

In the lower part of the channel, on the contrary, a region with a positive space charge will be formed, as evidenced by the fact that potential here will assume a positive value. It can be predicted that, under the action of primary and slow secondary electrons, a region with a potential gradient sufficient to accelerate ions in the direction of electron gun will be formed, and forming plasma will correspond in its characteristics (density and temperature) to a glow-discharge plasma. However, processes of ion acceleration simulation using the developed program, run on a computer with the above-cited characteristics, may take considerable time (up to several days). This is due to a significant difference in the masses of ions and electrons. The most obvious solution of this problem is transition to parallel computing technology.

4. Conclusion
1. It is shown that, using proposed complex physical and mathematical model, it is possible to study plasma formation process during the influence of electron beam on metals.
2. Analysis of the first simulation results has been carried out. There was shown a significant effect of ionization process on electric field distribution in gas-vapor channel. It was established that at the initial stage of the process, a region with a positive potential is formed in the lower part of gas-vapor channel, and in its upper part, on the contrary, potential decreases.
3. It is shown that for effective application of the developed model and studying of the drift process of metal ions, having a significant mass in comparison with electrons, using of parallel computing technology is necessary.

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