Optimization of the Current Density Distribution in Electrochemical Cells Based on the Level Set Method and Genetic Algorithm

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Abstract. This paper proposes a general applicable algorithm for the optimization of the current density distribution in the electrochemical cells using the insulating shields during the electroplating process. The innovative aspect is that the position of the insulating shield is displaced over a number of predefined time steps convecting its surface proportional with and in the direction of a well chosen rate provided by a genetic algorithm. The aim of this method is to develop a systematic modification of the insulating shield position in order to get a more uniform distribution of the current density, hence a more uniform deposited layer at the cathode. As the displacement of the insulating shield is performed with the Level Set Method, the re-meshing of the computational domain with finite elements is not required anymore. Finally an example related to the optimization of the current density distribution in the vicinity of a singularity (incident angle between the electrode and insulator = 180°), using an insulating shield will be presented.

Key words. current density optimization – genetic algorithm – potential model – moving boundaries – finite element method – coupled problems – level set method.

PACS. 02.60.Cb Numerical simulation; solution of equations – 02.70.Dh Finite-element and Galerkin methods – 41.20.Cv Electrostatics; Poisson and Laplace equations, boundary-value problems – 02.60.Pn Numerical optimization

1 Introduction

Progress in electrochemical science and engineering continues to have a pronounced impact on a variety of industrial processes, including electroplating and electrochemical machining, corrosion, microelectronics, energy storage, energy conversion, etc. There is an industrial growing demand towards increasing the performance of these processes. In order to meet the specifications and achieve the quality of the products, most of the time design of an electrochemical application is faced to extensive trial and error, involving huge human resources and a considerable time to market.

In order to ensure high efficiency and low costs, the design of the electrochemical cells is necessary to be optimized. This requires an understanding of the behavior of the electrochemical system in terms of current density, potential and concentration distribution on the electrodes and in the electrolyte solution. In addition to that, it is very important to have a quantified model that describes the performances of the electrochemical reactor and powerful software that allows to simulate the electrochemical processes going on. The ability to visualize, even if imperfectly, the potential field and consequently the current density distribution in the electrochemical reactor is a great aid in making favorable adjustments in the geometry of the setup.

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An electrochemical cell generally consists of electrodes immersed in ionic solutions bounded by insulators. When the electrodes are connected to an electrical energy source, the flux of the electrons from the outer circuit transforms into a flow of ions in the electrolyte. At the electrode surfaces, electrochemical reaction occur. The nature of the involved electrochemical processes is generally very complex. However several assumptions and simplifications of limited validity can be made in order to tackle the main aspects of the problem. For example, if the electrode reactions take place at low rates, such that the concentration gradients are neglected, the potential distribution may be found using Laplace's equation. As a consequence, the resulting model describes the ohmic effects in the electrolyte [1]. This model is referred to as the Potential Model (PM).

An early interest for modeling this kind of topics has been shown in several works. Several authors applied the PM to compute the current density distribution and hence the electrode growth rate for electroforming (EF) applications. Bergh and Alkire [2] applied the Finite Element Method (FEM) to solve the resulting Laplace equation, with nonlinear boundary conditions that account for electrode charge transfer reactions. Deconinck [3,4] discretized the equations of the PM using the Boundary Element Method (BEM) in order to compute the changing electrode profile for nonlinear boundary conditions. They also presented a complete study of the electrode shape change as a function of electrode reactor dimension for different angles between the electrode and an adjacent insulator. Using the Finite Difference Method (FDM), Bozzini

and Cavallotti [5] presented numerical simulations for the Chromium (Cr) plating process on corner-shaped cathodes. They incorporated effects of mass-transport in the boundary conditions of the potential model. Georgiadou et. al. [6, 7] studied copper deposition in a particular trench geometry. The simulation of the shape evolution is coupled with a FDM for solving diffusion governed transport in the trench. Qiu and Power [8] developed a boundary element scheme in order to solve the problem of electrode shape change in an electrochemical process involving convection, diffusion and migration. They paid particular attention to the role of each mechanism in determining the pattern of deposition by implying a B-spline function that represents the electrode at each time step.

In the electroplating cells, metal deposits are produced at the cathodes. The high nonuniform current density due to the edge effects on the sharp corners is transferred to a high nonuniform deposition layer, like in the case of Cr electroplating on a cogwheel (see figure 1 left). Managing a more uniform current density (e.g. applying a masking procedure based on the insulating shields), produces a more uniform Cr layer (see figure 1 right).

When the electrochemical cell optimization in terms of current density is required, the electrochemical problem to be solved becomes even more complex since the model needs to be combined with an optimization algorithm. This involves a repetitive calculation of the electrochemical problem for different configurations/parameters (shape and/or position of the constitutive elements, rec-

Fig. 1. Cr electroplating on a cogwheel: (left) high nonuniform Cr layer; (right) more uniform Cr layer due to the masking of the edge effects.

tifier parameters, electrolyte parameters, etc.) of the electrochemical reactor.

Most of the known works [17, 18, 21, 22] make use of the optimization methods for process parameter identification in the field of electrochemical applications, but literature is very scarce when position or shape optimization of the constitutive elements of an electrochemical cell is required.

Majority of the known techniques, in field of topology and/or shape/position optimization, are based on FEM and suppose a large number of mesh adaptations. Often such techniques end-up with the re-meshing of the entire computational domain. Making robust algorithms for topology and shape/position optimization tools, based on this approach, is still challenging e.g. keeping or mapping the computational mesh [17, 18]. The shape/position optimization techniques are based on an Euler scheme for the boundary displacement. The method derives from the Lagrangian approach of changing boundary problems that supposes the grid boundary is attached to the moving front. The method is not well suited to compute bifurcation fronts [24]. In addition, the method shows insta-

bility and oscillation problems, high deformation of the boundary elements and intrinsic inability to deal with the topology changes. In order to avoid the above mentioned problems, of the boundary perturbation, this paper proposes a moving boundary algorithm based on the Level Set Method (LSM) [9].

LSM has been already widely used in structural mechanics optimization applications. Sethian and Wiegmann in [10] presented a combined level set and finite difference technique for constructing efficient designs which satisfy certain design criteria like minimization of the material consumption under constant stress. Osher and Santosay used in [11,12] LSM in combination with projected gradient method [13], to construct a simple numerical approach for problems involving a vibrating system in structural engineering. Allaire et. al. proposed in [14] a systematic implementation of the LSM where the front velocity is derived from a shape sensitivity analysis in structural design for different objective functions in two and three space dimensions. Zhen Luo presented in [15] an effective parametric approach by extending the conventional LSM to structural shape and topology optimization using the compactly supported radial basis functions (RBF) and the optimality criteria method. They represented the structural design boundary implicitly as a zero level set function and applied the RBF to interpolate the level set function (LS).

In the field of electrical devices optimization LSM has been used by Purcar et. al. in [23] as a new approach

for the shape perturbation of the resistors with complex geometry.

In this paper the moving boundary algorithm based on LSM is demonstrated in combination with the genetic algorithm (GA) [20] for the position optimization of an insulating shield in an electrochemical cell, in order to get a more uniform distribution of the current density at the cathode (incident angle between the electrode and insulator = 180°) [24].

2 Mathematical model and solution method

The mathematical model consists of three coupled problems: an electrochemical computation problem, an optimization algorithm and a moving boundary problem. After the computation of the electrochemical model e.g. PM current density distribution is completely known at the studied electrode. The aim of finding a uniform current density distribution at the electrode refers to the minimization (or maximization) of a scalar function with GA. Based on the GA, LSM will provide the new position of the insulating shield. According to the new position the electric field is distorted resulting a more uniform distribution of the current density at the electrode.

2.1 Electrochemical model (Potential Model)

An electrochemical process occurs whenever an electric current flows between electrodes of an electrochemical reactor. The electrolyte is modeled as an electric field problem without charge distributions inside the domain and

nonlinear boundary conditions at the electrodes [2–4, 24]. This problem is governed by Laplace’s equation:

$$\bar{\nabla} \cdot (-\sigma \cdot \bar{\nabla} U) = 0, \quad (1)$$

where σ [$\Omega^{-1}\text{m}^{-1}$] and U [V] represents the conductivity, respectively the electrolyte potential.

The current density J [A/m²] at the electrode reduces to:

$$\bar{J} = -\sigma \cdot \bar{\nabla} U. \quad (2)$$

Note that in this case Ohm’s law holds and the conductivity does not need to be constant. Indeed, it is possible to couple domains with a different conductivity or systems with a local varying conductivity (e.g. function of T the temperature of the electrolyte in [K], $\sigma(T)$).

2.1.1 Boundary conditions

The boundaries conditions of equation (1) can be essentially divided into insulating walls (insulators) and electrodes. The reactor’s walls, as well as the gaseous medium in contact with the electrolyte, can be seen as insulators. No current flows through them, and therefore the normal current density at each point is zero:

$$J_n = \bar{J} \cdot \bar{1}_n = -\sigma \cdot \bar{\nabla} U \cdot \bar{1}_n = -\sigma \frac{\partial U}{\partial n} = 0. \quad (3)$$

where the subscript n refers the normal direction. The same boundary conditions can be applied to symmetry planes.

Depending on the working conditions the current density distribution can be presented using different expressions. One option is to use a linear relation

$$J_n = A(V - U - E_0) + B, \quad (4)$$

where A in [A/(Vm²)] and B in [A/m²] are the polarization constants. This is often expected when large current densities are applied at oxygen evolving electrodes due to the thin passivation layer [1–7].

For single metal deposition processes the current density distribution is often quite accurately described by a Butler-Volmer type relation [1–7].

$$J_n = J_0 \cdot \left(e^{\frac{\alpha_a F}{RT}(\eta - E_0)} - e^{-\frac{\alpha_c F}{RT}(\eta - E_0)} \right), \quad (5)$$

where J_0 is the exchange current density, α_a and α_c the anodic and cathodic charge transfer coefficients, R the gas constant in [Jmol⁻¹K⁻¹] and T the temperature of the electrolyte.

In the most general situation, the current density distribution is described as function of the metal potential V , the electrolyte potential adjacent to the electrode U , the equilibrium potential E_0 and the efficiency θ :

$$J_n = f(V, U, E_0, \theta). \quad (6)$$

This function is often obtained by measurements and approached with a spline function [2–7]. The PM cannot make distinction between parallel reactions. In order to consider these effects, it is necessary to provide addition information (such as the efficiency θ for gas evolving side reactions).

2.2 Optimization method

The GA is widely recognized today as a powerful stochastic optimization method. It became very popular through the work of Goldberg [19]. Topa and Munteanu used in

[21,22] the GA for the optimal design of electromagnetic devices. The same approach is recalled in this paper and is based on the mechanics of natural selection and genetics. The genetic operators acted on an initial population of individuals, in such a way that the newly created individuals had better performances than their predecessors. The advantages of GA methods consist in offering the possibility to:

- optimize a large number of design variables,
- optimize discreet parameters,
- perform a "global" optimization,
- optimization is performed without the computation of the gradients.

The main disadvantage of the GA method is the relatively large amount of the computation time as compared with the case when deterministic methods are applied, but this is compensated by the fact that it is not necessary to evaluate the corresponding derivatives (performing the sensitivity analysis). When using the numerical analysis method for the electrochemical problems computation such current density distribution, the sensitivity analysis can be very difficult and can induce specific numerical derivative errors that are avoided when the GA or any other stochastic methods are used.

Usually in a GA, the design variable vector $\bar{p}$ is represented by a (chromosome). The correspondence can be made in several ways, but the binary representation is used most frequently [21]. In this case, each byte represents the equivalent of a gene (L is the number of bits per chromosomes).

If, for example, the design variable vector consists of two variables $\bar{p}=\{p_1, p_2\}^T$ and 4 bits are used per variable, then a possible chromosome ($L = 8$) has the following form:

$$\begin{array}{llll} chromosome & \rightarrow & 1001 & 0001 \\ variable & \rightarrow & p_1 & p_2 \end{array} \quad (7)$$

An initial chromosome population associated to a design variables set is randomly generated at the beginning of the optimization process. The members of this population are called generically "parents". The following operators are usually defined in a GA method [20]: *reproduction*, *crossover*, *mutation*, *the fitness function* and *the stopping rule*. A special attention should be paid to the last two as they are responsible with the proper functioning of the GA.

The fitness function basically determines which possible solutions passes in order to be used into the next generation of solutions. It evaluates the chromosomes and makes some qualitative assessment, returning a fitness value for that solution.

The GA evolves selecting and reproducing parents until a termination criterion is met. Setting the maximum number of generations is one of the most frequent stopping criterion. Population convergence criterion can be also used as a termination strategy. In general, GA forces majority of the population to converge to a single solution. Termination condition is the sum of deviations of the individuals to be smaller than a specified threshold. The GA can also be terminated when, in the best solution over a specified number of generations, no improvement occurs.

The GA can be summarized as follows:

- Step 1:* Codify the optimization problem design variables into a chromosome;
- Step 2:* Define the fitness function, and specific parameters of the genetic operators: reproduction, crossover, mutation and the stopping rule;
- Step 4:* An initial population of chromosomes is randomly generated;
- Step 5:* Each chromosome is decoded and the fitness function is evaluated;
- Step 6:* A new population is created with the reproduction, crossover and mutation operators;
- Step 7:* If the stopping rule is achieved then stop. Else go to step 4.

2.3 Boundary displacement model (Level Set Method)

LSM tracks the whole moving boundary, with a rate $\bar{v}$ (speed) normal to every point, function of a well chosen law, equation (12), provided by the GA. LSM uses the boundary shape change rate in the following convection equation:

$$\frac{\partial \Phi}{\partial t} + \bar{v} \cdot \nabla \Phi = 0. \quad (8)$$

2.3.1 Level set principles

The partial differential equation (8) defines the motion of the interface $\Phi(\chi, t) = 0$ through a grid, $\chi = (x, y)$ in $\mathbb{R}^2$, that is fixed in space with the velocity $\bar{v}$ defined at every grid point. This equation represents the Eulerian formulation of the interface evolution being captured by

the implicit function $\Phi(\chi, t)$ than tracked by interface elements as it was calculated in the classical Lagrangian formulation equation [9, 10].

Let us consider a closed moving interface $\Gamma(t)$ in $\mathbb{R}^2$ and $\Omega(t)$ a region (possibly multi-connected) that is enclosed by $\Gamma(t)$ and that moves with a constant velocity $\bar{v}$ normal to the interface as in figure 2 left.

Fig. 2. Left: zero contour of Φ representing the front Γ at $t=0$ (—) and two possible interface evolutions $\Gamma(t...)$ and $\Gamma(t-...)$; Right: the signed distance function representation (surface $-\Phi$) and zero LS.

Supposing that (χ, t) is a particle trajectory on the interface $\Gamma(t)$, the implicit function $\Phi(\chi, t)$, called the zero LS function which represents at each moment the location of the interface $\Gamma(t)$, is defined as follows:

$$\begin{cases} \Phi(\chi, t) < 0, & \text{in } \Omega(t) \\ \Phi(\chi, t) = 0, & \text{on } \Gamma(t) \\ \Phi(\chi, t) > 0, & \text{in } \mathbb{R}^2 - \Omega(t) \end{cases} \quad (9)$$

There are many possibilities to express $\Phi(\chi, t)$, but in most of the LS applications it is described as:

$$\Phi(\chi, 0) = \pm d, \quad (10)$$

where "d" is the so-called signed distance function (SD), the distance from the interface $\Gamma(0)$ to every point of do-

main $\mathbb{R}^2$. This ensures that the interface $\Gamma(t)$ is represented by the zero LS, see figure (2) right.

When the function $\Phi(\chi, t) = 0$ is derived by applying the chain rule [25], the following equation is obtained:

$$\frac{\partial \Phi}{\partial t} + \sum_{\chi} \underbrace{\frac{\partial \chi}{\partial t}}_{\bar{v}} \cdot \frac{\partial \Phi}{\partial \chi} = 0, \quad (11)$$

Equation (11) in fact is the same as equation (8) and demonstrates how the implicit representation of a curve is related to the motion of this curve.

2.3.2 Boundary displacement rate

The LSM requires velocity $\bar{v}$ to be known at least on the moving boundary. In order to find the optimal position of the insulating shield, the boundary displacement rate is quite simple computed and given by:

$$\bar{v} = \frac{\bar{p}_2 - \bar{p}_1}{dt} \quad (12)$$

where $\bar{p}_1$ and $\bar{p}_2$ are two consecutive positions of the insulating shield and the time dt can be arbitrarily chosen.

2.4 Numerical solution method

2.4.1 Potential model

To reduce the continuum problem described by equation (1) to a discrete system of algebraic equations, the standard FEM is used. The definition domain Ω of equation (1) is discretized into elements (triangles). The FEM formulation for the Laplace equation (1) on the domain can be

written as in [16]:

$$\sum_{N_{el}} \left[\int_{\Gamma_{el}} N_i \left(\frac{\partial N_k}{\partial x} n_x + \frac{\partial N_k}{\partial y} n_y \right) d\Gamma_{el} - \int_{\Omega_{el}} \left(\frac{\partial N_k}{\partial x} \cdot \frac{\partial N_i}{\partial x} + \frac{\partial N_k}{\partial y} \cdot \frac{\partial N_i}{\partial y} \right) d\Omega \right] \cdot U_k = 0 \quad (13)$$

N_i , N_j and N_k are respectively the weight and shape functions, $i, j, k = 1, 2, 3$ (the vertices of the triangles), Γ_{el} is the boundary of the element and Ω_{el} that part of the domain Ω (in 2D a surface) occupied by an element. Equation (13) can be rearranged for all nodes k of Ω_{el} in the following system of equations:

$$[K] \cdot \{U\} = \{F\}, \quad (14)$$

with $[K]$ the system matrix, $\{U\}$ the vector of unknown potentials in the nodes and $\{F\}$ the first term of equation. The introduction of proper boundary conditions makes the system of equations unique. When the equation (4), is used as boundary condition, equation (14) can be directly solved. Otherwise the righthandside of equation (14) becomes nonlinear at the electrode boundaries (nonlinear boundary conditions of type (5) and (6)) and an iterative, Newton-Raphson process is used in order to obtain the solution.

2.4.2 Level set method

– Signed distance function and velocity extension

Common choice for the SD function is the solution of the Eikonal equation $|\nabla \Phi| = 1$ with boundary condition $\Phi = 0$ (the zero LS function which coincides with $\Gamma(0)$). This method is in literature also referred to as the Fast Marching Method (FMM) [9]. The FMM first initializes

the points that are adjacent to the interface with the minimum distance between these points and the interface. Using these adjacent points as boundary condition for the Eikonal equation, the final solution is found by upwind differentiation on the whole computational domain. The above mentioned procedure is used in our implementation.

Since the LSM only needs to be effective for the $\Phi = 0$ isocontour, equation (11) is not necessary to be integrated on the entire computational domain. The integration algorithm perfectly fits if it is applied on a narrow band around the interface $\Gamma(0)$. The computation of the narrow band is performed during the SD computation step. Using FMM, all triangles in certain distance from the moving interface are marked. The narrow band width is usually computed as the product between the maximum velocity v_{max} at the moving front and the total LS process time T_{LSM} . Here the narrow band is chosen in such way not to be larger than 10 layers of triangles.

Velocity distribution from the moving interface Γ to the LS computation region is called the "velocity extension". Sethian used the FMM for the velocity extension [9]. The method applied in this work is similar to the one in [9], and uses the narrow band extrapolation.

– *Numerical Integration*

In order to find the new shape and position of the insulating shield, equation (11) is numerically integrated in space and time with initial conditions as governing equation (10) and with a velocity defined at every grid point. The majority of the LSM applications are based on the Cartesian grids [9,12]. In this work, a triangular unstruc-

tured mesh, the same as for the FEM analysis is used for the numerical integration of the LS equation [27].

Equation (11) is discretized using the residual distribution formulation with the standard Galerkin finite element shape functions and multidimensional upwind method [25, 26]. In order to distribute the residuals to triangle vertices a Low Diffusion A scheme (LDA) have been used [26]. The time integration is approached using a second order accurate Petrov-Galerkin (PG) formulation. The set of equations derived from (11) can be written as:

$$\overline{\overline{M}} \left\{ \frac{\partial \Phi}{\partial t} \right\} + \overline{\overline{C}} \cdot \{\Phi\} = 0, \quad (15)$$

where: $\left\{ \frac{\partial \Phi}{\partial t} \right\}$ is the vector of the time variation of Φ in each node $[Nx1]$, $\{\Phi\}$ is the vector of the unknowns at each time step $[Nx1]$, $\overline{\overline{M}}$ is the global mass matrix $[NxN]$, $\overline{\overline{C}}$ is the global convection matrix $[NxN]$.

One of the LS demands for such time domain integration scheme is that the scheme must follow some underlying properties as consistency and monotonicity, which are substantial in the integration of the LS equation. These criteria are fulfilled by combining LDA scheme for space integration and PG formulation with mass matrix stabilization $\overline{\overline{M}}$ for the time integration [26].

The new position of the interface is found by interpolating the solution, $\Phi(x, y, t)$, of equation (11) on the FEM mesh.

It is important to be mentioned that while the interface $\Gamma(0)$ convects towards a new position and shape also the triangular elements enclosed by the new interface must be always updated with all the properties (e.g. conductivity) of the elements at the old position of $\Gamma(0)$. This updating

is of outmost importance in the resolving of the coupled PM problem with the right material and boundary conditions.

– Time step definition

The integration of equation (15) requires that the total process time T_{LSM} is divided into a number of time steps Δt_{LSM} . The time step definition is further related to the re-initialisation of the LS equation to the SD function. The concept of re-initialisation is a powerful numerical tool in the LS theory and it has been extensively discussed in [9]. The time step Δt_{LSM} is chosen such that the front crosses no more than one grid cell of size h each time step:

$$\max ||\bar{v}|| \Delta t = h, \quad (16)$$

where the maximum is chosen from all values of $\bar{v}$ at all possible mesh points in the narrow band.

3 Numerical results

The computational environment used in this work is object oriented and it has been developed in house by the authors. It can handle any shape of 2D single or multiple domain geometries which are defined in SolidWorks and discretized with an unstructured triangular mesh [27]. The computation of the equation systems (14) and (15) is implemented both for an iterative and direct LU solver (<http://www.boost.org/>).

The example presented in [24] for the copper EF in the vicinity of a singularity (incident angle between the electrode and insulator surface = 180°) is analyzed in this

work for the optimization of current density distribution (hence layer thickness). LSM in combination with the GM described in [19] is used to compute the position of an insulating shield in order to smooth the current density along the whole cathode length. The insulating shields are widely used in electroplating to improve the performances of the electrochemical reactor. By positioning an insulating screen between the electrodes, the electric field is distorted such that an uniform distribution of current density occurs at the electrode under consideration.

3.1 Model Definition

The electroplating cell as used in the experimental set-up of reference [3,24] is given in figure 3 left. The distance between the cathode and anode is 120 mm. The length of the cathode and anode is 199 mm, respectively 307 mm and the reactor's width 7.9 mm. An insulating screen, $40 \times 8 \times 7.9$ mm, is introduced in-between the electrodes 50 mm from the cathode, 15 mm from the left side of the electroplating cell, see figure 3 right. The electrolyte

Fig. 3. Geometry of the electroforming reactor in the vicinity of the singularity.

consists of a $CuSO_4$ solution. The specific conductivity of the electrolyte is $\sigma_1 = 23.2 \Omega^{-1} m^{-1}$ and the electrode

polarization (6) behavior have been measured at 25°C [3, 24]. The insulating shield is modeled as second domain with conductivity $\sigma_2=1.0\text{e-}6\Omega^{-1}\text{m}^{-1}$.

The electrochemical problem is approached with the PM which is characterized by the Laplace equation (1) with non-linear boundary conditions (6). The following phenomena will be taken into account:

- ohmic drop in the electrolyte solution;
- anodic polarization.

A 2D computational domain is defined using a cross-section through the reactor in figure 3, by a plane perpendicular to the middle of the electrodes. Using the FEM, the governing Laplace equation with non-linear boundary conditions is solved for each "optimal" position of the insulating shield in order to get the normal current density distribution J_n at the cathode surface. A detailed solution convergence study for both electrochemical and electrode shape change model has been presented in [24].

In order to accurately compute the current density distribution around the singularity, but also to ensure a high accuracy in the moving of the insulating shield over the triangulated domain, a very fine mesh of 37,322 points and 73,788 elements is constructed. The normal current density distribution along the developed cathode length is plotted in figure 4 for the initial position of the insulating shield. At the cathode-insulator junction the edge effect produces an initial current density peak of -542 A/m^2 .

Fig. 4. Current density distribution along the cathode (singularity located at 199 mm).

3.2 Optimization

Figure 5 shows the flow chart of the developed computing environment base on GA as optimization tool and LSM as moving boundary algorithm.

Fig. 5. Flow chart of the solving environment using the GA method.

Table 1. GA specific parameters

Number of design variables	2
Number of chromosomes per individual	4
Length of a chromosome	8
Number of individuals per generation	10
Crossover (p_c) probability	0.8
Mutation (p_m) probability	0.08
Lower limit of the design variables (x, y) [mm]	1, 1
Upper limit of the design variables (x, y) [mm]	266, 11
Ending criteria	f(j) ≤ 10%
or the maximum number of generations = 2000	

The main idea is to change the design variable vector $\bar{p} = \{x, y\}^T$ such that the standard deviation equation (17) of the current density distribution at the cathode surface to be minimal.

The fitness function is chosen as a measures of the calculated current density J_i , at each grid point of the cathode, function of the mean value J_{avg} :

$$f(J) = \sqrt{\frac{\sum_{i=1}^n (J_i - J_{avg})^2}{n - 1}}, \quad (17)$$

The values of the GA parameters used during the optimization process are specified in table 1. They have been attentively selected during the numerical tests in [21,22] for the best convergence rate to the optimal solution.

Most of the practical electroplating applications consider the current density distribution at the cathode surface being uniform when its standard deviation is smaller than 10%. The same ending criterion is applied to the GA but also the maximum number of generations is imposed.

Using the FEM, LSM equation is solved in order to compute the new shield position. In case of position optimization, which does not involve any topological changes, velocity extension as described in [23,24] is not necessary anymore, and is directly calculated from the final and initial vector position of the insulating shield equation (12) for an arbitrarily $dt = 1$ s.

LSM only on a narrow band of triangles around the moving front [9] (see figure 6 left) is solved. After the initialization (and reinitialisation) of the LS function Φ with the SD function, LS equation (15) is iterated over the narrow band (see figure 6 right). The usual number of triangles taken in the narrow band during LS displacement is c.a. 3,490 elements (c.a. 1,790 points) and considerably reduces the computational effort of LS equation (15). The

Fig. 6. Narrow band around the moving boundary(left); zoom of the narrow band and the SD function from the boundary of the shield representation $d = -2, 0, 2$ and 4 mm (right).

microscale time step Δt_{LSM} is accordingly computed such that it stays within the narrow band. LS equation is integrated implicitly within roughly 5 to $10 \approx t_{LSM}$ time steps. The new zero LS solution gives the new position of the insulating shield for the next optimization time step. As v_{max} is subject to changes at the next optimization step, for every GA individual generation Δt_{LSM} and the narrow band are accordingly updated.

The distribution of the potential field on the computational domain in figure 6 is found from the equations(1- 6) and represented in figure 7 by zero LS for the initial position of the insulating shield (top) and for the optimal position of the insulating shield (bottom).

Fig. 7. Potential field for the starting position of the shield; position of the shield is given by the zero LS function (top); Potential field for the optimal position of the shield; position of the shield is given by the zero LS function (bottom).

The initial standard deviation of current density at the cathode (17) is 70%. After 110 generations, see figure 8, it decreases to 8%.

Fig. 8. The evolution of the objective function.

The best parameters of the shield position are obtained for $x = 184$ mm and $y = 10$ mm, see figure 9. A comparison

Fig. 9. The final position of the insulating shield.

between the current density distribution for the initial and optimal shield position is represented in figure 10.

Fig. 10. Current density distribution along the cathode for the initial and final position of the shield.

3.3 Computational specifications

Calculation times are c.a. 2 minutes for each of generation resulting a total computational time of 230 minutes. The calculations have been carried on a PC Pentium 4, 2.4 GHz, 2 GB RAM.

4 Conclusions

This paper proposed a general applicable numerical algorithm for the optimization of the current density distribution using the insulating shields during the electroplating process in an electrochemical reactor. The mathematical model used for the shape optimization consisted in three coupled problems, an optimization, an electrochemical and a moving boundary problem. A standard GA algorithm provides the optimal position of the insulating shield. The electrochemical problem uses PM to compute the current density distribution at the electrodes. PM is discretized with the standard FEM. The moving boundary problem, which updates the position of an insulating shield, hence material properties within the interface, is a result of the integration of the LS equation. LSM has the strong feature that it does not need remeshing of the computational domain after the changing of the insulating shield position and it shows the real benefit especially when is coupled with a GA. In order to highly accelerate the optimization procedure, the LS equation is not solved on the whole FE mesh of the computational domain but on a narrow band of FE elements around the insulating shield interface. Residual distribution formulation, LDA, combined with second order PG is used for the space respectively time integration of the LS equation. The results obtained are very encouraging and the procedure described can be applied, in principle, to even more complex problems. Therefore, the ongoing work will be extended to also handle shape optimization problems.

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