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Potentials of the phase field approach for modeling modifications in material microstructure during Electrical Discharge Machining

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Abstract

Electrical discharge machining (EDM) can be classified as a manufacturing process with main thermal active principle. During this process the induced thermal energy on the material leads to numerous surface modifications such as metallurgical transformation, tensile stresses or initiation of micro cracks. These modifications on the surface can strongly affect the functionality of the produced component. Simulation of microstructure modifications during EDM can be a beneficial approach in prediction of surface modifications and consequently, variations in material properties. Phase field approach which has been emerged during last twenty years, is well known as a powerful method in modeling microstructure evolution. Models based on this approach describe microstructure modifications in mesoscale. This paper investigates the potential of phase field approach for modeling of microstructure evolution in EDMed surfaces and subsurfaces.

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Keywords: EDM, Phase field modeling, Simulation, Material modification, Microstructure evolution

1. Introduction

Prediction of component functionalities such as durability, reliability, and fatigue life has always been one of the main concerns in manufacturing technology. As it is well known by now, functionality and properties of a component are directly affected by its surface quality and surface modifications [1–3]. Plastic deformation, initiation of microcracks, phase transformation, variation of residual stresses and variation of micro hardness can be named as common surface modifications [4]. Surface modifications are in turn result of microstructure evolutions during each process [5]. Thus, in order to construct a comprehensive model for prediction of material and surface modifications during a process, simulation of microstructure evolution should also be considered.

Electrical discharge machining (EDM) is a thermal process with complex material removal sequence including heating up the material to evaporation temperature and its resolidification with high cooling rates [1,6]. EDMed surfaces are normally covered with a recast layer (WL) caused by resolidification of remained molten material. This recast layer, which is non-etchable is known as white layer. Directly beneath WL, heat affected zone (HAZ) can be observed. In HAZ solid-state phase transformation occurs as the temperature exceeds the phase transformation temperature [7–9]. EDM process like other thermal processes leads to tensile residual stresses on the surface. As a result of these tensile stresses, microcracks may initiate within the white layer [1,10].

Similar to other manufacturing processes, numerous investigations on the surface modifications during EDM have been performed [1,8,11–13]. Contrarily to the considerable number of experimental studies on this matter, only few investigations on modeling and simulation of microstructure modification and surface modification during EDM can be found in literature. The lack of literature on this subject can partially be explained by the complexity of microstructure evolution in EDM. This complexity is a result of high local

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temperatures and temperature gradients applied on the material during EDM.

However, recently studies on the modeling of microstructure evolution during welding process based on phase field approach have successfully been carried out. As EDM and welding have considerable similarities relating to their physical active principle this circumstance motivates similar studies for EDM. For this reason in this paper after a review on the phase field models introduced for welding processes, the possibility of implementing similar models for EDM is discussed.

2. Phase field Modeling

2.1. Microstructure, and microstructure evolution

Microstructure refers to different inhomogeneity, appearing in the structure and composition of material as a result of material processing. The inhomogeneity can include phases differing in composition or crystal structure, grains with different orientation, local defects such as dislocations and pores, etc. This definition normally considers the structural aspects in intermediate mesoscale. Microstructure evolution occurs as the material tries to reach its minimum value for free energy [3].

2.2. Phase field theory

The conventional methods used in modeling of microstructure evolution are phenomenological approaches, which consider the grains of structural or compositional domain as mathematically sharp interface. In these approaches the interfacial velocity is considered as a boundary condition. In models based on conventional approaches the interface position should be accurately determined. However, determination of interface position is not an easy task especially in complex 3D models. Moreover, this question can always be posed: "how the interfacial surface should be viewed" [3,14].

In last twenty years, phase field approach gained lots of attention among material scientists. Models based on this approach are able to describe different types of microstructure evolution such as, solidification, solid-solid transformation, grain growth, crystal growth, surface stresses, dislocation movements, and crack propagation.

Phase field approach is based on the idea of diffuse-interface introduced by Cahn & Hilliard [15]. According to this idea, the densities of extensive quantities change with slight gradient from their value in one phase to new value in another phase trough the interfacial zone [3]. In this approach temporal evolution of microstructure is described by Cahn-Hilliard nonlinear equation of diffusion [16] and Ginzburg-Landau phase transition theory [17].

Phase field models can be categorized in two types. In the first one, the phase field variable ϕ is introduced as an additional variable. By using this new variable tracking of the interfacial zone can be avoided. The second type, which is broadly used in the modeling of solid-solid phase transformations, considers a well-defined physical parameter as a phase field variable. This variable can be a long range parameter or a compositional field variable [3].

Phase field theory describes the evolution of microstructure in binary systems. Steinbach et al. [18] have extended the phase field approach to solve multiphase systems. In this approach each phase or grain is identified by an individual field variable. The evolution equation for multiphase systems can be obtained from minimization of free energy functional. The simplified model of evolution equation for multiphase system can be written as:

$$\frac{d\phi_i}{dt} = \sum_{j \neq i} \mu\sigma \left[\left\langle \phi_j \nabla^2 \varphi_i - \varphi_i \nabla^2 \phi_j \right\rangle - \frac{\pi^2}{2\eta^2} \left(\varphi_i - \phi_j \right) \right] \quad (1)$$

Where φ_i, ϕ_j are phase field parameters respective to phase i and j, σ is the interfacial energy, μ is the interfacial mobility and η refers to the interfacial boundary thickness [5].

2.3. Phase field models for manufacturing processes with main thermal active principle

EDM along with welding and laser processes are categorized under the class of manufacturing processes with main thermal active principle. In the mentioned processes thermal energy is applied as the main factor in order to modify components. Due to the analogous active principle among these processes, in many cases they evoke similar mechanisms for modification of material, especially for comparable thermal cycles. In general it can be proven that the material is only sensitive to the combination of applied loadings, independent from the process itself [19,20].

For simulation of processes such as welding and EDM as well as laser hardening or laser welding, the effect of a localized heat source on the material should be modeled. The proposed models simulate the applied thermal energy independent from the sort of generation. In other words, the models do not simulate the plasma channel in EDM, electric arc in arc welding or laser beam in laser welding or laser hardening, but they model the effect of generated heat on the material. Hence, a model which introduced for simulation of one process with main thermal active principle may be transferrable to other processes with similar active principle. However, the model may need considerable modifications due to differences between processes. These differences have to be considered in the boundary conditions. As a result, for simulation of material modification during processes with similar active principles in macro and microscale, relatively similar principles can be used. Therefore, a review on phase field models proposed for other thermal processes is assumed to be a good starting point for construction of similar models for EDM.

There have been some investigations concerning simulation of microstructure evolution of material during different types of laser processes such as laser hardening

[21,22]. However, to the best of the author's knowledge no comprehensive study on microstructure evolution of material based on phase field theory can be found in literature for laser processes. Contrary to EDM and laser processes, different studies on the phase field modeling of microstructure evolution during welding process have been published. In following section studies on microstructure evolution based on phase field approach during welding processes are discussed in detail.

3. Phase field models for welding

Welding is one of the most common joining methods applied on steels. The induced thermal loadings on the material during welding processes lead to numerous modifications on the microstructure of material [23]. Often the active mechanisms in the microstructure of HAZ of welded components such as phase transition, grain growth lead to weak mechanical properties in this region. Therefore, simulation of microstructure evolution during this process can be beneficial for controlling the microstructure evolution and, thus properties of components [24]. Thiessen el. al. in series of publications [23, 25] introduced a physical model based on phase field theory to describe the microstructure evolutions in HAZ of welded components. In their first work from this series of studies [25], Thiessen et al. simulated the microstructure evolution for AISI 316L (DIN X2CrNiMo19-12) steel during welding as well as different heat treatments. In the proposed model, they defined the interfacial velocity by considering the movement of interface of phases in molecular scale. Using this approach, Thiessen et al. were able to calculate the interactional velocity mostly by using typical mechanical properties of material such as shear modulus, yield stress, burgers vector, etc. However, for achieving more accurate results they had to take the crystallization temperature and nucleation density from experimental data.

Using the proposed physical model Thiessen simulated the microstructure evolution during gas tungsten arc welding (GTA). Within this study, the current, voltage and welding velocity were set to 35 A, 10 V and 2 (mm/s). Experiments as well as simulations were performed for three different samples with different heat treatment histories and, consequently different initial microstructure. The samples included, the so called as received samples which were subjected to stress relief and stabilized heat treatment (SRS), the partially heat treated samples which were gone under additional heat treatment and the annealed samples. Further, the austenite grain growth during mentioned heat treatments and (GTA) welding process was simulated. Comparing the results of simulation with the experimental data from welded samples showed that the predicted grain sizes in HAZ of partially heat treated samples are smaller than the grain sizes measured from the welding experiment. For the as received sample the results of simulation turned to be more realistic. In addition, presented results of microstructure simulation during a welding cycle showed that the distribution of recrystallized domains is not homogeneous in the material. The first recrystallized domains nucleates along the grains or triple junctions.

Within the same series of studies [23] austenitization and retransformation of austenite to ferrite for low carbon steel AISI 1005 (DIN DC05) during a welding process were simulated. In this model Thiessen et al. used the TCFE2 database and ThermoCalc® to construct the phase diagram for Fe-C. By applying the mentioned diagrams, determination of A1- and A3-temperatures were possible. Thiessen et al. implemented the thermodynamic data into phase field code named MICRESS®. This phase field code is based on the multiphase approach introduced by Steinbach et al. [26].

Furthermore, for modeling of nucleation during heating and cooling process the nucleation temperature was calculated by using the critical nucleation parameters and finite superheating. While the nucleation density was obtained by applying the information extracted from post and pre-micrographs of the partially transformed zone. Implementing the mentioned information to the phase field model, microstructure evolution during (GTA) welding was simulated. The welding current for this process was considered to oscillate between 90 and 130 A, while the welding voltage and velocity were set to 17.5 V and 0.6 (mm/s).

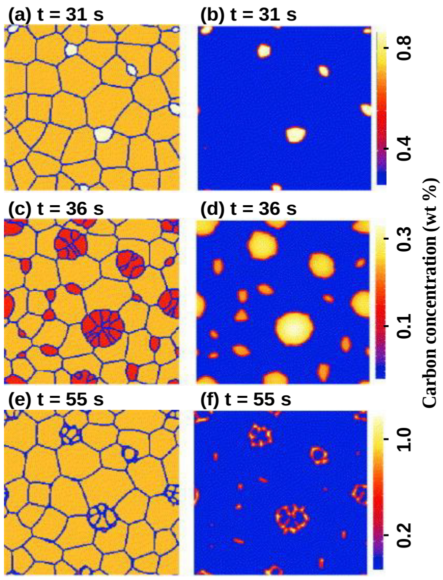

Fig 1. Phase evolution during a welding cycle. (a), (c), and (e) Perlite phases are illustrated in white, austenite in red and ferrite in yellow. (b), (d), and (f) carbon concentration (wt %) during welding cycle [23].

Result of simulation during a welding cycle for AISI 1005 (DIN DC05) steel is illustrated in Fig. 1. According to simulation results, in this steel grade as well as in AISI 316L (DIN X2CrNiMo19-12) nucleation occurs along the grains and triple junctions Fig. 1(c). It can also be observed from the simulation that the concentration of carbon in most austenite phases is homogenous. Nevertheless, some regions contain noticeably high carbon concentrations, Fig. 1(d). Following, as the temperature of material decreases to temperatures under

A3, austenite transforms into ferrite. During cooling carbon restricts the ferrite grain growth and forms small carbon rich regions, Fig. 1(e) and (f).

ased on the same approach as the works presented by Thiessen et al., Toloui et al. [27] investigated the austenite grain growth during the arc welding of X80 steels. In this study, the authors considered the effect of alloying particles on the austenite grain size. According to simulation results, during cooling process, depending on the peak temperature of the thermal cycle different mobility behaviors could be observed. Temperature peaks lower than dissolution temperature of alloying particle (NbC) result in low mobility during cooling and vice versa. Subsequently, by implementing periodic thermal boundary condition on the microstructure domain, simulation of microstructure evolution in heat affected zone has been performed. This simulation illustrated the grain growth with respect to distance from the center of fusion zone. According to the results of simulation, proposed model was successful in describing the austenite grain growth by reducing the distance from the center of fusion zone.

Last important work discussed here in detail concerning microstructure simulation of welding, has been presented by Ramazani et al. [24]. In this work the microstructure evolution for Dual Phase steel (DP) during gas metal arc welding was investigated. Like previous examples in this study the thermodynamic data was obtained from thermodynamic data base, while the mobility coefficient and nucleation density were obtained by fitting the simulation results for phase fraction and grain growth with the dilatometric results.

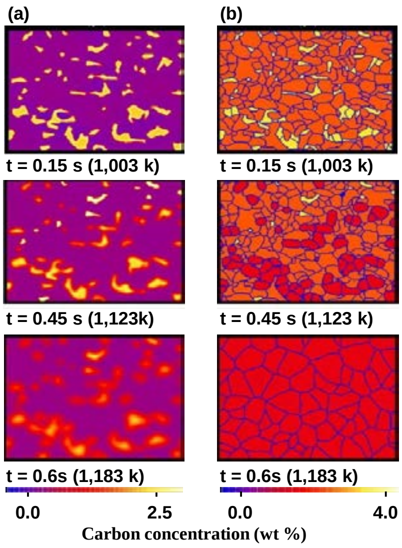

Fig. 2 (a) the evolution of carbon concentration (wt %), (b) the phase transformation to austenite, yellow illustrate martensite, orange ferrite and red austenit [24].

Furthermore, the carbon diffusion was coupled to the grain growth simulation, while other alloying particles were assumed to be immobile. Simulation of cooling process has been performed for different cooling rates. The austenite-bainite transformation was only considered during cooling process, where the bainite nucleation temperature was obtained from experiments. It was also assumed that the remained austenite transforms to martensite. For high cooling rates compared to low cooling rates, higher austenite/bainite interface mobility, and greater amount of nuclei were considered. The result of simulation for phase fraction during heating process was found to be in agreement with experimental data. In addition, the proposed model was able to simulate the nucleation of austenite phase into the martensite phase and the austenite grain growth up to consumption of whole martensite, Fig. 2.

Microstructure evolutions has also been simulated for two different temperature peaks (1,350 °C and 1,050 °C) and two different heating rates (400 °C/s and 100 °C/s) Fig. 3. According to the results of these simulations, for higher temperature peaks larger austenite grains can be expected Fig 3(a) and (b), while higher heating rates lead to smaller austenite grains for identical temperature peaks, Fig 3(a) and (c).

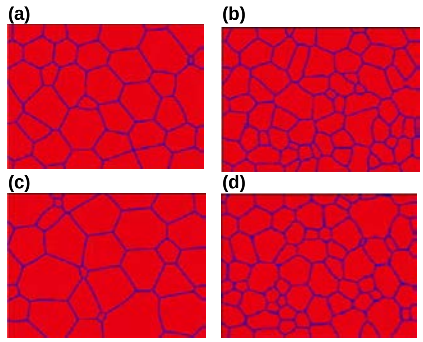

Fig. 3 Final austenite grain structure for different temperature peaks and heating rates (a) 1,350 °C, 400 °C/s; (b) 1,050 °C, 400 °C/s; (c) 1,350 °C, 100 °C/s; (d) 1,050 °C, 100 °C/s, [24].

In addition to the studies discussed in detail during this section, there are other published investigations in literature on modelling of microstructure evolution for welding. As an example, work by Apel et al. [28] should be mentioned. In this study the phase field transformation in the HAZ of welded X65 steel in line pipe was simulated. In another investigation by Montiel et al. [29] solidification of binary alloy (magnesium AZ31) in the welded zone was modeled. The focus of this study was the transformation of columnar to equiaxed dendrites during resistance spot welds. Farzadi et al. [30] also modeled the weld pool solidification of molten Al-Cu alloy during (GTA) welding using phase field approach.

4. State of the art in modeling microstructure evolution and surface modifications in EDM

As discussed before, only few investigations on microstructure evolution during EDM processes can be found in literature. In this chapter some of these efforts for modeling surface and microstructure modifications are summarized. Additionally, the limitations and weak points of existing models in comparison to phase field models are briefly discussed.

Das et al. [10] and Perez et al. [31] separately modeled the evolution of residual stresses and the formation of crater shape during EDM processes with relatively similar models. Both models are based on finite element method and consider simulation domains in the order of 10^{-3}m. In the model proposed by Das et al. [10], different regions such as molten regions and HAZ are recognized by using the simulated nodal temperature data through the material. In order to model the material removal during the process, some elements were eliminated from the molten region during the simulation. The remaining material was assumed to be solidified to martensite phase due to high cooling rates. For simulation of the residual stresses in this model, elastic and plastic properties of material were considered as temperature dependent functions. To define this dependency, authors used experimental results from literature. The shrinkage of material in crater area was simulated as a result of removed elements. Further, by keeping the high pressure boundary condition during the whole discharge duration, the high shear stresses around the crater formed its typical edge.

In the work introduced by Perez et al. [31] evolution of microstructure fractions for AISI 4140 (DIN 42CrMo4) steel during EDM process was simulated. In this study the necessary thermal boundary conditions for modelling of microstructure evolutions have been obtained from the simulation results and experimental measurements. By implementation of the temperature data to the non-equilibrium approach, phase fractions in rim zone have been calculated. For this objective, the authors used the CALCOSOFT^{TM} software. In non-equilibrium approach the kinematics of phase transition can be solved for different thermal histories by using thermodynamic diagrams. Using this method, prediction of white layer width and thickness of heat affected zone was possible. Subsequently, authors calculated the thermal stresses and the stresses induced by the phase transition to martensite on the surface of material. Transformation to martensite phase results in 4 % local volume expansion of material and, consequently, in appearance of moderate compressive stresses on martensitic zones. Moreover, by taking the effect of martensite formation into account, a high shear stress zone between white layer and HAZ has been predicted by the simulation.

The reviewed studies by Das et al. and Perez et al., which try to model the effect of phase transition on the material modifications, are limited to calculation of the variations in phase fraction around the rim zone. None of these models is able to give information about the topography evolution of microstructures, orientation of phases, crystallization, grain growth and dislocation densities, etc. As mentioned before in this paper these properties play an important role in the functionality of the manufactured component.

There were also variant studies using the molecular dynamic (MD) approach in modeling of surface properties such as residual stresses and crater formation for micro- and nano-EDM [32–36]. Models based on molecular dynamics may give a valuable insight about the stress evolution and creation of crater but due to the difference in spatiotemporal scale for MD and EDM these models are limited to simulation of micro- and nano-EDM. Furthermore, these models do not give information about the phase changes. Thus, as these studies are not included in the scope of this paper they are not further discussed.

5. Transferring the phase field models proposed for welding processes to EDM

By using phase field models effect of important factors such as thermal pinning, concentration of alloying particles and the initial topography of microstructure can be taken into consideration. Phase field models discussed here reveals the abilities of these models in simulation of microstructure evolutions during processes with main thermal active principles. As mentioned before, these models do not simulate the plasma channel, or electric arc, but they model the effect of thermal energy on the material modifications. Due to this fact, the models introduced for welding can be transferred to other processes with main thermal active principles or at least they can be the basis for construction of suitable models for these processes. However, the differences between processes should be considered during transferring such models (e.g. differences between welding and EDM). This can be done by application of suitable boundary conditions and performing the necessary modification on the model.

Some important differences which should be considered during modelling of EDM can be named as follows. In general, discharge durations in EDM are in order of µs which is obviously shorter than thermal cycle durations in arc welding. EDM includes formation of plasma channel while in welding electric arc appears during the process. In welding thermal energy is applied on the larger area of workpiece in comparison to the area affected during a single discharge in EDM. Moreover, EDM is a process with discontinues thermal loadings when in many cases the thermal load applied during welding is continues. In addition, welding normally is done in presence of shielding gas which prevents the welded material from oxidation, while EDM process normally is performed in a fluid medium. This differences lead to different boundary conditions in simulation of microstructure evolution during EDM process.

6. Summery

Simulation of microstructure evolutions during EDM process can help in predicting and controlling the microstructure evolution in HAZ. Thereby, controlling or even adjusting defined material modifications may become possible. Despite of great potentials of such models no comprehensive microstructure model for EDM can be found in literature. However, phase field models introduced recently for analogue processes can give insight to similar studies for EDM.

In this paper after a brief introduction to phase field approach in modeling of microstructure evolutions and processes with main thermal active principle, phase field models proposed in literature for welding processes have been reviewed. Further, the state of the art in modeling of surface modification for EDM has been reviewed. Finally, possibilities and challenges of transferring the phase field models proposed for welding to EDM processes have been demonstrated and critically discussed.

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