# Study of the machining process of nano-electrical discharge machining based on combined atomistic-continuum modeling method

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## ABSTRACT

Nano-electrical discharge machining (nano-EDM) is an attractive measure to manufacture parts with nanoscale precision, however, due to the incompleteness of its theories, the development of more advanced nano-EDM technology is impeded. In this paper, a computational simulation model combining the molecular dynamics simulation model and the two-temperature model for single discharge process in nano-EDM is constructed to study the machining mechanism of nano-EDM from the thermal point of view. The melting process is analyzed. Before the heated material gets melted, thermal compressive stress higher than 3 GPa is induced. After the material gets melted, the compressive stress gets relieved. The cooling and solidifying processes are also analyzed. It is found that during the cooling process of the melted material, tensile stress higher than 3 GPa arises, which leads to the disintegration of material. The formation of the white layer is attributed to the homogeneous solidification, and additionally, the resultant residual stress is analyzed.

## 1. Introduction

As a non-touching machining method, due to its high machining accuracy and broad machining spectrum of materials, electrical discharge machining (EDM) has been widely used in manufacturing industry, especially in the fields referring to hard-to-machine materials or parts with demands of complex shape or high precision. With the need of modern industry and cutting-edge technologies for ultraprecise and nanoscale parts is becoming more and more pressing, new technologies about EDM have been developed to extend the dimension range of EDM to nanometer scale in recent years. For example, using the capacity coupled pulse generator Kunieda et al. [1] developed a device for nano-EDM with which the discharge duration was less than tens of nanoseconds and discharge craters with a diameter of as small as 570 nm were obtained. Using a ultrasmall-diameter tool electrode for machining is another way for nano-EDM. Egashira et al. [2] drilled holes with a diameter of less than 1 μm in zinc using a silicon tool electrodes with a diameter of less than 0.15 μm. Another new technology for nanofabrication which is termed as nano electrical machining (nano EM), though more like nano-EDM [3], and in some literatures is definitely identified as nano-EDM [4,5], is developed. In this

technology, to get an extremely accurate control of the motion of electrodes, equipment like atomic force microscope (AFM), scanning tunneling microscope (STM), and so on which are capable of accurate motion control are utilized to get a gap of several nanometers in length between the two electrodes [3,5,6]. Using this method, the diameter of obtained craters can be as small as tens of nanometer.

Nano-EDM can be seen as nanoscale EDM, and their fundamental processing mechanisms are similar. Nevertheless, owing to the complexity and randomicity of EDM, the regime of mechanism of EDM is still incomplete, and so is that of nano-EDM. To better understand the mechanism of EDM and improve the EDM technology and related technologies, for example, nano-EDM, lots of researches on the mechanism of EDM have been conducted. In EDM, the discharge channel in which complex physical and chemical phenomena take place is the driver of EDM process, therefore experimental studies, computational simulation studies and theoretical studies of the mechanism of EDM are mainly focused on the discharge channel. The spectroscopy was used to study the discharge channel experimentally [7,8]. In these experiments, high-speed video camera was used to photograph the arc plasma (AP) in EDM, and then the temperature distribution in the AP was depicted by the line pair method. It was found that temperature in the center of the AP can rise to between 4000 K and 8000 K, and the diameter of the AP is about five times of that of the crater. By applying analysis of optical emission spectroscopy to the EDM plasma, an

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insight into the mechanism of the AR was given in [9]. As for the nano-EDM, though its fundamental processing mechanism is similar to that of EDM, some characters of nano-EDM are different from that of EDM. According to [5], different from that of EDM, in nano-EDM, the work function of electrode material has no effect on the breakdown process of dielectric, field-emission-assisted avalanche in nanoconfined liquid dielectrics is believed to be the main reason leading to the breakdown process, and additionally, the electrical field required for nano-EDM is 66 times stronger than that for EDM. As for the material removal mechanism of nano-EDM, several models were proposed [3,5,10,11]. Typically, the electron deposited thermal energy leads to the ionization of the dielectrics in the gap, and a current with extremely high current density forms between the two electrodes. A great amount of thermal energy is produced owing to this current, which will cause the heating, melting, vaporizing and eventually ablation of the material. Numerical study is another effective way to reveal the mechanism of EDM. Most of these numerical models are based on the heat transfer theory, especially for the two electrodes [12–14], while for the discharge channel, hydrokinetics model or electricity model are integrated into the heat transfer model [15,16]. It should be noticed that in these models all or part of the material at a temperature higher than the melting point is considered ablated. Under this assumption, some characteristics of EDM were represented, for example, the influence of processing parameters on the shape of crater and the topography of the EDMed surface, the energy distribution, the material removal rate, and so on. However, in these continuum models, the dynamics behaviors of material was not considered, which makes it hard for these models to describe the phenomenon related to material dynamics in EDM, such as the process of material ablation and the evolution of material microstructure.

Molecular dynamics simulation (MDS) works at atomic level. MDS allows for dynamics simulation of material and its quantities have explicit physical meanings, which makes it an effective way to study material characters and behaviors in material processing from the atomic point of view. Lots of applications of MDS to laser machining have be reported [17–20], medicine research [21,22], and so on. Recently, study about micro-EDM with MDS is conducted by Yang et al. [23], however, in their model, electron heat conduction (EHC) which plays the predominant role in heat conduction in metal was neglected, which will inevitably lead to some discrepancy between the simulation results and the reality. Except [23], few papers about EDM with MDS has been reported as the authors know. To take into account the effect of electron heat conduction to better describe the heat transfer process while maintaining the capacity of dynamics description of MDS, a combined atomistic-continuum modeling method was proposed [24]. In this method, the atomistic molecular dynamics simulation model (MDSM) and the continuum two-temperature model (TTM) are integrated using a coupling term by which the deposited thermal energy to the lattice system from the electron system in the TTM are transferred to an additional momentum-dependent force imposing on each atom in the MDSM. This method inherits the advantages of both the TTM and MDSM, and it is quite suitable for the modeling of the nano-EDM process.

In this paper, we establish a simulation model for single discharge machining process in nano-EDM by the combined atomistic-continuum modeling method. Based on this computational simulation model, the melting, disintegrating, ablating and solidifying processes of material in single discharge are presented and analyzed to get an insight into the machining process of nano-EDM. The sketch of this paper is as follows. In Section 2, the principle of the combined atomistic-continuum modeling method are reviewed, and details of the modeling process are elaborated. In Section 3 results from the simulations are presented, and based on those simulation data the mechanism of nano-EDM is analyzed.

In the last section, the simulation results and analysis are briefly reviewed, and a discussion about the model and the mechanism of nano-EDM is made.

## 2. Modeling

### 2.1. Combined simulation model

It is hard to agree with the simulation conditions using traditional continuum simulation methods, for example the finite difference method, the finite element method, or atomic simulation methods such as the MDS method alone in studies of the nano-EDM mechanism. For one thing, the simulation dimensions are nanoscale, and the dynamics effect of material is also required, both of which are beyond the simulation scope of continuum simulation methods; for the other thing, violent thermal inequilibrium exists between the electron system and the lattice system in heat transfer process in metal, which leads to the unsuitability of MDS. To settle the similar problems as those confronted here, Ivanov and Zhigilei [24] proposed a combined simulation method integrating the TTM and the MDSM. This method is applied to our model to settle the problems aforementioned.

#### 2.1.1. Two-temperature model

To deal with the femtosecond-scale heat conduction, TTM was proposed [25,26]. In the TTM, the electron system and the lattice system are taken as two separated thermal systems in each of which a heat transfer process goes on. The interaction between the two system is described by adding an extra position-dependent 'heat source' whose intensity is determined by the temperature deviation between the two systems at the interested site to each system. Mathematically, according to the TTM the heat conduction process can be expressed as the following two coupled equations,

$$C_e(T_e)\frac{\partial T_e}{\partial t} = \nabla[K_e(T_e, T_l)\nabla T_e] - G(T_e - T_l) + H_e(\mathbf{r}, t), \qquad (1)$$

$$C_l(T_l)\frac{\partial T_l}{\partial t} = \nabla[K_l(T_l)\nabla T_l] + G(T_e - T_l) + H_l(\mathbf{r}, t), \qquad (2)$$

where $C$ is the heat capacity, $K$ the is thermal conductivity, $G$ is the electron-lattice coupling factor, $H$ is the heat resource, and $\mathbf{r}$ is the position vector, while the subscripts $e$ and $l$ denote the corresponding material parameters and variables of the electron system and the lattice system respectively. The heat conduction model of each separate system is nearly of the same formation as that in Fourier heat transfer theory except for the electron-lattice coupling term, namely, the second term on the right side of Eqs. (1) and (2). $C$ and $K$ are both temperature-dependent theoretically, however, in practise reduction is often applied to them. For electron system, it is generally adopted that $C_e$ is linearly related with the temperature, namely, $C_e(T) = \gamma T$. As for $K_e$, its precise formation is complicated as presented in Ref. [27], nevertheless, in calculations performed with TTM, it is often expressed as

$$K_e = K_0 \frac{T_e}{T_l} \quad , \qquad (3)$$

where $K_0$ is the thermal conductivity when $T_e = 300\,\text{K}$ and $T_l = 300\,\text{K}$.

For the lattice system, the expressions of $C_l$ and $K_l$ is relatively simple. Due to the fact that the characteristic time of the lattice system is much smaller than that of the electron system, its temperature evolution is quite slow compared to that of the electron system. Thus, $K_l$ is often taken as a constant. Additionally, considering that the heat conduction process of the lattice system is always neglected for simplicity, we get $K_l = 0$. The interaction between the two systems corresponds to the second term on the left side of Eqs. (1) and (2), in which $G$ determines the interaction strength.