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Modeling of reactive kinetics in the metal surface contaminant cleaning using atmospheric pressure plasma arc

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ABSTRACT

Atmospheric pressure plasma arc (APPA) cleaning is a newly developed method of metal surface cleaning. In this paper, a mathematical model of reactive kinetics in the metal surface contaminant cleaning using APPA has been developed. Based on the analysis of APPA cleaning mechanism and the feature of cleaning interface, a governing equation was established with heat transfer equation and energy conservation on the moving interface. Using fourth-order Rounge–Kutta method, above equation was solved and removal percentages of the cleaning contaminant at different time were obtained. In virtue of reactive kinetics theory, a reactive kinetics model of metal surface cleaning using APPA was established on the base of above calculation results. Afterwards, reactive kinetics parameters such as activation energy and pre-exponential factor were calculated. Cleaning lubricant was taken as an example, the results indicated that predictive values of lubricant removal percentages gotten from this established reactive kinetics model show good consistent with experimental data at the same time. Furthermore, the ambient temperature on the cleaning lubricant surface affects the removal rate strongly. The removal rate increases with the increase of the ambient temperature. To avoid the damage of metal substrate surface because of higher temperature and ensure the removal rate of the lubricant, the appropriate temperature which lies between the lubricant decomposition temperature and damage temperature of metal substrate under given calculation conditions should be determined.

1. Introduction

Metal sheets are generally covered with slushing oils for temporary corrosion protection or with lubricants for friction reduction during metal-forming process. These organic films have to be removed before further surface finishing of the metal sheets [1,2]. However, conventional cleaning methods such as mechanical cleaning, wet chemicals cleaning and ultrasonic cleaning [3] usually require direct contact or the intervention of external agents which can lead to additional contamination or damage of treated surfaces.

As a new alternative cleaning method, atmospheric pressure plasma arc (APPA) cleaning [4–6] can overcome the cited drawbacks of conventional cleaning methods and vacuum limitation of low-pressure plasma cleaning [7]. APPA focuses on the sample surface and generates energy density enough to induce physical and chemical reactions such as thermal shock, activation decomposition, thermal expansion and spalling. The activation decomposition plays a key role in the cleaning process. In addition, the thermal shock of arc energy flow, thermal expansion and spalling can remarkably improve cleaning contaminant capability of the activation decomposition. As a result, an ablation of the contaminant takes place at any selected cleaning field. Furthermore, different materials can be cleaned by choosing proper arc energy density without the damage of metal substrate.

By analyzing the mechanism of APPA cleaning, it can be concluded that there is a moving cleaning interface along contaminant thickness direction which changes computational domain and nonlinear boundary condition. Unfortunately, except that Kim et al. [8] investigated the effect of pulsed power of DBD on the removal rate using a phenomenological model, few investigations [9] attempt to quantitatively study the mechanism of APPA cleaning metal surface using mathematical models. This makes the research on APPA cleaning have to depend on experiments or personal experience. The model of APPA cleaning contaminant from metal surface is established using reactive kinetics theory based on the mechanism and features of APPA cleaning in this paper. The intrinsic relationships between contaminant removal percentages, removal rate and influencing factors are revealed. The

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effect of the ambient temperature on the cleaning surface to the contaminant removal rate is investigated.

2. Modeling approach

2.1. Treatment of hot source

In the process of metal surface cleaning using APPA, the arc can be regarded as a moving hot source. With the movement of hot source on the sample surface, the energy density of APPA follows Gaussian distribution in its column section [10], which can be written as

$$q_{\mathrm{r}} = \frac{4P}{\pi d^2}\exp\left(\frac{-4r^2}{d^2}\right) \tag{1}$$

where q_{r} is the arc energy density in column section, P is the effective power of plasma arc (it also included other plasma effects), $4P/\pi d^2$ is the power density in the center of plasma arc, d is the nozzle diameter and r is the distance of a spot in column section to center of the arc.

For simplifying the calculation, average heat flux of the plasma arc column section is treated as input parameter, which can be obtained from

$$q_{\mathrm{m}} = \left(1 - \exp\left(\frac{-4r_0^2}{d^2}\right)\right)\frac{P}{\pi r_0^2} \tag{2}$$

where r_0 is the diameter of arc column section. Eq. (2) is regarded as the expression of plasma arc hot source and is introduced into the heat transfer equation according to the boundary condition of constant heat flux density. The arc column continuously scanning on the cleaning surface can be simulated with short steps, intermittent and jumping movement, whose step is the diameter of arc column section in each hot source moving.

2.2. Governing equation of moving cleaning interface

In the process of APPA cleaning, besides the energy density of heat source, the material characteristics and thermal properties of contaminant cleaning all have impact on its removal rate. Irradiated by APPA, the contaminant come into being activation decomposition and temperature gradient occurs in the contaminant. In this process, there is a moving cleaning interface along contaminant thickness direction. Applied this feature and the characteristic about approximate constant heat flux density on the cleaning surface into heat transfer differential equation of the contaminant, a governing equation of moving interface is established.

Furthermore, it also can be considered that cleaned production immediately disengages from the moving interface. Moreover, a portion of APPA heat energy irradiating on the cleaning surface is transferred from the cleaning interface to the contaminant interior. At the same time, the other heat energy is transformed into decomposition heat and dissipated from the moving cleaning interface. Afterwards, it can be regarded that heat transfer implement along the contaminant thickness direction due to its temperature gradient occurring along heat flux direction. Consequently, heat transfer equation of the contaminant can be expressed as

$$\rho c\frac{\partial T}{\partial t} = \lambda\frac{\partial^2 T}{\partial x^2} \tag{3}$$

where ρ is the density of cleaning contaminant, T is the temperature, t is the time, c and λ is the specific heat, the thermal conductivity of cleaned contaminant, respectively.

The initial conditions are as follow: $t = 0, T = T_0, 0 \le x \le L$. where L is the thickness of the contaminant.

Due to the whole process of APPA cleaning being divided into pre-heating stage when surface temperature reaches decomposition temperature of the contaminant and cleaning stage when the contaminant is being eliminated, the boundary conditions consist of that in each stage.

Boundary condition in the pre-heating stage can be expressed as

$$x = 0, \quad \lambda\left(\frac{\mathrm{d}T}{\mathrm{d}t}\right)_{\mathrm{top}} = -q_{\mathrm{m}}; \qquad x = L, \quad \lambda\left(\frac{\mathrm{d}T}{\mathrm{d}t}\right)_{\mathrm{bottom}} = 0.$$

Boundary condition in the cleaning stage can be expressed as

$$x = S(t), \quad T = T_{\mathrm{r}}; \qquad x = L, \quad \frac{\mathrm{d}T}{\mathrm{d}t} = 0$$

In addition, in the cleaning stage, it conforms to the rule of energy conservation on the cleaning interface, which is written as

$$q_{\mathrm{m}} = \left(-\lambda\frac{\partial T}{\partial x}\right)_{x=S} + \rho\,\Delta h\frac{\mathrm{d}S}{\mathrm{d}t} \tag{4}$$

where $S(t)$ is the displacement of cleaning interface, T_{r}, Δh are the decomposition temperature and activation decomposition heat of contaminant, respectively.

With Fourier series law [11], analytical solution of the differential equation in the first stage of APPA cleaning is written as

$$T = T_0 + \frac{q_{\mathrm{m}}L}{\lambda} \times \left\{\frac{1}{3} + \frac{at}{L^2} - \frac{x}{L} + \frac{x^2}{2L^2} - 2\sum_{n=1}^{\infty}\frac{1}{(n\pi)^2}\cos\left(\frac{n\pi x}{L}\right)\exp\left(-at\left(\frac{n\pi}{L}\right)^2\right)\right\} \tag{5}$$

where a is the coefficient of temperature conductivity, which is expressed as

$$a = \frac{\lambda}{\rho c} \tag{6}$$

When the contaminant is heated to its decomposition temperature and the second stage starts, temperature distribution of the contaminant can be obtained from

$$T = T_0 + \frac{q_{\mathrm{m}}L}{\lambda} \times \left\{\frac{1}{3} + \frac{at_{\mathrm{r}}}{L^2} - \frac{x}{L} + \frac{1}{2}\frac{x^2}{L^2} - 2\sum_{n=1}^{\infty}\frac{1}{(n\pi)^2}\cos\left(\frac{n\pi x}{L}\right)\exp\left(-at_{\mathrm{r}}\left(\frac{n\pi}{L}\right)^2\right)\right\} \tag{7}$$

where t_{r} is the time from initial temperature to decomposition temperature, which is get from

$$T_{\mathrm{r}} = T_0 + \frac{q_{\mathrm{m}}L}{\lambda}\left\{\frac{1}{3} + \frac{at_{\mathrm{r}}}{L^2} - 2\sum\frac{1}{(n\pi)^2}\exp\left(-at_{\mathrm{r}}\left(\frac{n\pi}{L}\right)^2\right)\right\} \tag{8}$$

Afterwards, θ, X and y_{l} are introduced and represents $(T - T_{\mathrm{r}})$, $(X - S)$ and $(L - S)$, respectively. With Fourier series law, analytical solution of heat transfer differential equation in the cleaning stage of APPA cleaning is expressed as

$$\theta(X, t) = \sum_{m=1}^{\infty}\frac{2\sin(\beta_{\mathrm{m}}X)}{y_{\mathrm{l}}}\exp(-at\beta_{\mathrm{m}}^2)\psi(m, y_{\mathrm{l}}) \tag{9}$$

where

$$\beta_{\mathrm{m}} = \frac{(2m-1)\pi}{2y_{\mathrm{l}}} \quad m = 1, 2, 3, \ldots$$