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Global sensitivity analysis of nanomachining parameters by using dynamic scanning thermal microscope

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ABSTRACT: In this study, global sensitivity analysis of nanomachining parameters by using a dynamic scanning thermal microscope is investigated. Thus, the cross-section of a nanomachined sample by sweeping with different tip radius on the vibrational response of the system at different speeds and temperatures are simulated. It is shown that by increasing temperature, the depth of nanomachining decreases, and by increasing tip radius, the depth of nanomachining increases. Also, it is declared that the final quality of the nanomachining decreases by increasing speed traveling. Then, the Sobol indices for the mean depth and surface finish of the nanomachined sample are studied. It is shown that traveling speed is not affected the mean depth of nanomachining in its physical range and so the effects of the probe traveling speed and interaction between parameters are negligible. It is declared that the effect of interaction between temperature, traveling speed and tip radius is important on the final surface finish of the sample, however, the most important parameter is still the temperature difference. Then, the total indices and Sobol indices are compared. It is stated that the total indices are significantly higher than the Sobol indices for the final surface of the nanomachining. For the mean depth of the nanomachining the total indices and Sobol indices for temperature and tip radius are approximately equal and the effect of probe traveling speed is negligible.

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1- Introduction

Scanning probe microscopes have different types, designed to achieve different goals according to their mechanism. One of these types of microscopes is scanning thermal microscope [1]. Due to the thermal mechanism in this type of microscopes and the possibility of using this term to melt the sample, these types of microscopes can be used for the nanomachining of nanoscale pieces [2].

Global sensitivity analysis was performed to investigate the effects of input parameters on one or more outputs. When all input factors change simultaneously, the global sensitivity is evaluated and the sensitivity within the entire range of each input factor is evaluated. This analysis can identify the contribution of different inputs in the output results and determine the extent of influencing each of the input parameters both independently and as an inter-parameter interaction on the output of the system. One type of global sensitivity analysis method is the variance-based Sobol method [3], which measures the sensitivity of the output to an input variable, relative to the amount of variance in the system output which caused by the input.

The main purpose of this study is to investigate the effects of temperature, tip radius, and traveling speed to better control the depth of nanomachining and increase the final surface of the nanomachined sample using global sensitivity analysis inspired by the basic excitation technique. In this analysis, the temperature distribution along the probe is done according to the linear temperature distribution function [2]. Assuming basic excitation, a mathematical model using Hamilton's principle and the equation of modes shape using the method of separating variables is available in the technical literature [4]. Therefore, the nonlinear partial differential equations of the dynamic scanning thermal microscope are solved analytically [5], using the assumed modes method [6]. The cross-section of a nanomachined sample is simulated by sweeping the tip with different radii on the absolute vibrational response of the system at different speeds and temperatures, and the depth and the final surface nanomachined are investigated. Finally, using global sensitivity analysis, the amount of direct effects and the interaction of each of the parameters of temperature, tip radius, and traveling speed, on the two outputs, the average depth and the final surface of the nanomachining are evaluated by the Sobol method.

2- Mathematical Model

A dynamic scanning thermal microscope probe with base excitation is studied in the non-contact mode and far away from the sample surface. The probe is assumed rectangular and uniform (width b and height h) with length L [2,4]. The schematic of the problem is shown in Fig. 1.

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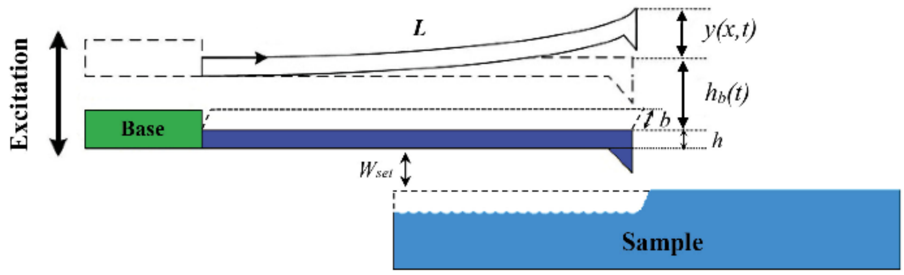

Fig. 1. Schematic of scanning thermal microscope probe configuration with base excitation.

The equation of motion and the boundary conditions of the problem are derived from the reference [4] based on Euler-Bernoulli beam theory and Hamilton's principle.

2-1- Assumed modes method

The assumed modes method [6] is used to solve the governing equations for the base excitation. The mode shapes mentioned in reference [4] are used as assumed modes of problem.

$$y(x,t)=\sum_{i=1}^{m} Y_i(x)q_i(t). \tag{1}$$

m is an integer, and it is clear that increasing m causes more accuracy of the method. $Y_i(x)$ are the equations of the mode shapes and $q_i(t)$ are the general coordinates of the problem. By solving the governing equations by Cramer's method, the public and private answers of the system are obtained as follows.

$$q_h^l=\sum_{i=1}^{m} r_{il}A_i^l\cos(\omega_{sh}^i t+\phi_i). \tag{2}$$

$$q_p^l=A_e^l\cos\omega_e t. \quad l,i=1,2,\dots,m \tag{3}$$

$A_i^l A_i^l$ ، $\phi_i\phi_i$ ، $A_e^l A_e^l$ are equal to the response amplitude $q_h^l q_h^l$ in $\omega_{sh}^i \omega_{sh}^i$, the response phase $q_h^l q_h^l$ in $\omega_{sh}^i \omega_{sh}^i$ and the amplitude at the base excitation frequency in $q_p^l q_p^l$, respectively.

The answer of the total system will be as follows:

$$q_t^l=q_h^l+q_p^l. \quad l=1,2,\dots,m \tag{4}$$

By applying the initial conditions in Eq. (4) and solving the resulting system of equations, the amplitude of the response at the shifted resonance frequencies of the 1st mod is obtained as follows:

$$A_{sh}^l=\sum_{i=1}^{m} r_{li}A_i^1. \quad l=1,2,\dots,m \tag{5}$$

The equations of relative vibration, absolute vibration and set point of probe are defined as follows:

$$\begin{aligned} y&=\sum_{l=1}^{m}(q_h^l+q_p^l),\\ y_{total}&=y+h_b,\\ y_{set}&=y_{total}+w_{set}.\\ l&=1,2,\dots,m \end{aligned} \tag{6}$$

where y is the relative vibration, $y_{total} y_{total}$ is the absolute vibration and $w_{set} w_{set}$ is the set point of probe adjustment.

۲-۲- Global sensitivity analysis by Sobol method

The mathematical model of scanning thermal microscope with base excitation is a model with nonlinear behavior and when the model is nonlinear, output analysis of variance can be used to analyze the problem [۷]. The model input vector for Z is specified as the system output in Eq. (۷).

$$\begin{aligned} Z&=f(\vec{\Psi})=f_0+\sum_{i=1}^{d} f_i(\Psi_i)\\ &+\sum_{i<j}^{d} f_{ij}(\Psi_i,\Psi_j)+\dots+f_{123\dots d}(\vec{\Psi}). \end{aligned} \tag{7}$$

$$\vec{\Psi}=(\Psi_1,\Psi_2,\dots,\Psi_d)\in R^d. \tag{8}$$

The analysis of variance function for the output is available as follows, which is called the numerical analysis function.

$$\begin{aligned} Var(Z)&=f_0+\sum_{i=1}^{d} D_i(Z)\\ &+\sum_{i<j}^{d} D_{ij}(Z)+\dots+D_{123\dots d}(Z). \end{aligned} \tag{9}$$

$$D_i(Z)=Var\left[\mathrm{E}(Z\mid\Psi_i)\right]. \tag{10}$$

$$\begin{aligned} D_{ij}(Z)&=Var\left[\mathrm{E}(Z\mid\Psi_i,\Psi_j)\right]\\ &-D_i(Z)-D_j(Z). \end{aligned} \tag{11}$$

where E is defined as a mathematical symbol.

To obtain the higher-order interaction, a mathematical process similar to Eqs. (١٠) and (١١) is used to obtain Sobol indices or sensitivity indices based on variance [٣].

$$S_i = \frac{D_i(Z)}{Var(Z)}, S_{ij} = \frac{D_{ij}(Z)}{Var(Z)}, \ldots \tag{12}$$

where $S_i S_i$ and $S_{ij} S_{ij}$ are equal to the input Sobol index i and the interaction index of the inputs, respectively. The number of

definable indices is equal $2^d - 1$. Total indicators or total effects are introduced as follows:

$$S_{(i)}^{tot} = S_i + \sum_{j \neq i} S_{ij} + \sum_{j \neq i, j \neq k, j < k} S_{ijk} + \ldots = \sum_{l \in \# i} S_l . \tag{13}$$

$S_{(i)}^{tot} S_{(i)}^{tot}$ represents the total index for the i input, which is obtained from the sum of the input Sobol index with the interaction index of the inputs. $\#i$ contains all subsets of the input parameter and its interaction with other parameters.

3- Results and Discussion

Fig. 2 of the nanomachined cross-sectional simulation shows a sample with 100 nm thickness in the base excitation mode with a linear Temperature distribution. By sweeping the tip radius on the absolute vibration response of the system, the simulated nanomachining profile is shown. The results show that the final surface and depth of the nanomachining increase by increasing the tip radius. Also, as the speed of the probe increases, the final surface decreases due to the increase in the variance of the absolute vibration response. By deeper examination of the simulations, it can be seen that the increase in temperature cannot be expressed alone as a definitive criterion for increasing the final nanomachined surface.

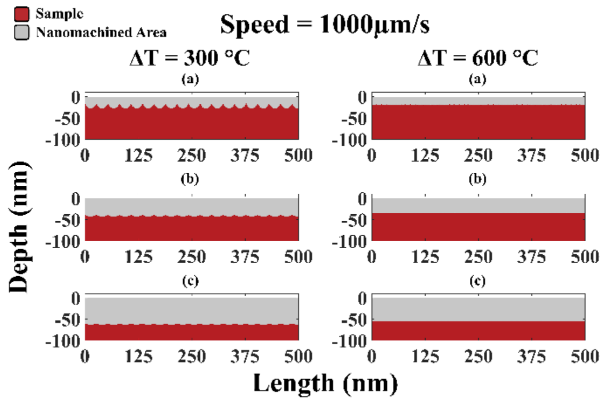

Fig. 2. Comparison of nanomachined final surface with base excitation at 300 °C and 600 °C at tip radius (a) 5nm, (b) 20nm, (c) 40nm and at speed of 600

By examining Sobol indices and total indices, the amount of direct effects as well as the interaction of each of the input parameters of temperature, tip radius and traveling speed on the two outputs, average depth and the final surface of nanomachining is determined. The results show that 2 parameters of temperature and tip radius on the average depth and all 3 parameters of temperature, tip radius and traveling speed on the final surface of nanomachining have a serious effect.

Figs. 3 and 4 show the effects of the input parameters both individually and as a sum of individual effects with inter-parametric interaction, for both outputs, average depth and smoothness of the final nanomachining surface. For example, the Sobol temperature index with 30/73% effect and the total temperature index with 84/74% effect, indicate that temperature independently 30/73% has an effect on the final surface and 51% is affected by the interaction between temperature and other parameters. This analysis is also available for both tip radius and traveling speed parameters.

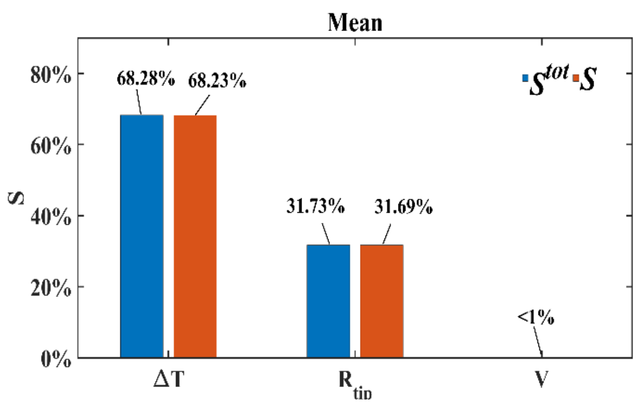

Fig. 3. Comparison of the effects of total indices and Sobol indices on the average depth of nanomachining.

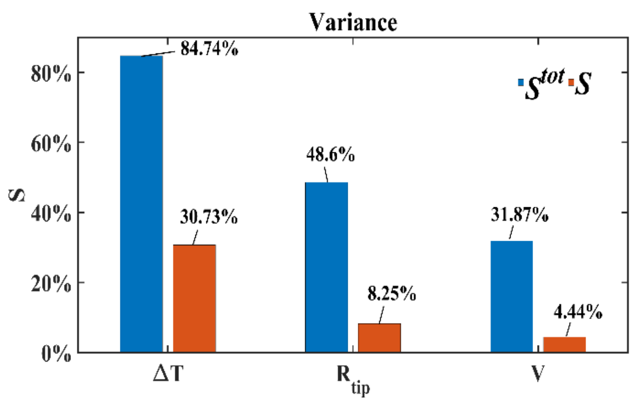

Fig. 4. Comparison of the effects of total indices and Sobol indices on the final surface of nanomachining.

4- Conclusions

By simulating the cross-section of a nanomachined sample, it was shown that increasing the tip radius increases the depth of nanomachining and increasing the traveling speed of the probe reduces the final surface of nanomachining. It was found that increasing the temperature does not necessarily improve the surface smoothness of the sample and temperature alone is not the only parameter affecting this issue. By examining the Sobol indices, it was shown that the effects of probe speed and interaction between parameters on the average depth of nanomachining can be neglected. It was also stated that in addition to the significant effect of inputs on the final surface of nanomachining, the interaction between these parameters is very effective. Finally, the effects of each input parameter on nanomachining outputs showed that the amount of total indices is significantly higher than Sobol indices in relation to the final surface of nanomachining, but in relation to the average depth of nanomachining, both indices for two parameters of temperature and tip radius are approximately equal and very insignificant for the probe speed.

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