ФИЗИКА

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ИССЛЕДОВАНИЕ ОБРАБОТКИ ПОЛИКРИСТАЛЛИЧЕСКИХ CVD-АЛМАЗОВ НАНОСЕКУНДНЫМ ЛАЗЕРОМ С ИСПОЛЬЗОВАНИЕМ НЕЧЕТКИХ МОДЕЛЕЙ

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INVESTIGATION OF POLYCRYSTALLINE CVD DIAMOND PROCESSING BY NANOSECOND LASER PULSES USING FUZZY MODELS

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Аннотация. Выполнено исследование процесса обработки поликристаллических CVD-алмазов импульсным наносекундным лазерным излучением и разработана интеллектуальная система прогнозирования геометрических параметров формируемых микроструктур с использованием аппарата нечеткой логики. Экспериментальные исследования проводились с использованием Nd:YAG лазера с длиной волны 532 нм. В качестве варьируемых параметров выступали количество импульсов, энергия импульса и диаметр лазерного пучка. Для построения модели использовался алгоритм нечеткого вывода Мамдани, реализованный в среде Python. Матрица планирования эксперимента формировалась на основе гранецентрированного центрального композиционного плана. Установлено, что в исследуемом диапазоне параметров обработки удаление материала происходит преимущественно за счет термомеханического разрушения и графитизации, что приводит к нелинейному росту размеров кратера при многоимпульсном воздействии. Разработана нечеткая модель, связывающая режимы обработки с глубиной и шириной формируемых лунок. Проверка адекватности модели показала достаточно высокую точность аппроксимации: коэффициент детерминации на тестовой выборке составил 0,7906 для глубины и 0,7940 для ширины лунки. Средняя абсолютная процентная ошибка (MAPE) на тестовой выборке не превысила 12,5%. Предложенный подход позволяет эффективно прогнозировать результаты лазерной обработки сверхтвердых материалов, минимизируя объем дорогостоящих натурных экспериментов.

Ключевые слова: *CVD-алмаз*, *наносекундные импульсные лазеры*, *лазерная обработка*, *нечеткое моделирование*.

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Abstract. This paper presents a study of the polycrystalline CVD diamond processing using pulsed nanosecond laser radiation and the development of an intelligent system for predicting the geometric parameters of the resulting microstructures based on fuzzy logic. Experimental investigations were carried out using an Nd:YAG laser with a wavelength of 532 nm. The variable parameters included the number of pulses, pulse energy, and laser beam diameter. The Mamdani fuzzy inference algorithm, implemented in Python, was used to construct the model. The experimental design matrix was based on a face-centered central composite design. It was established that within the investigated range of processing parameters, material removal occurs primarily due to thermomechanical fracture and graphitization, leading to nonlinear crater growth under multi-pulse exposure. A fuzzy model was developed to relate the processing conditions to the depth and width of the resultant cavities. The model validation revealed a reasonably high approximation accuracy, with a coefficient of determination of 0.7906 for the depth and 0.7940 for the width on the test set. The mean absolute percentage error (MAPE) on the test set did not exceed 12.5%. The proposed approach enables effective prediction of laser processing outcomes for superhard materials, hence reducing the necessity for expensive physical experimental tests.

Keywords: *CVD diamond*, *nanosecond pulsed lasers*, *laser processing*, *fuzzy modeling.*

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Introduction

Polycrystalline CVD (Chemical Vapor Deposition) diamonds are recognized as highly promising materials in contemporary industry, attributed to their unique combination of physical and mechanical properties. These characteristics render them suitable for applications in advanced technology sectors, including cutting tool manufacturing, optics, and electronics. The physical and mechanical properties of diamond, which provide advantages as

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a structural material, also present technological challenges in its processing. Conventional diamond processing techniques exhibit low productivity, significant tool wear, and restricted ability to create complex geometric shapes. Simultaneously, laser cutting offers non-contact, high-precision, and controlled interaction with the workpiece material. Nanosecond lasers represent a distinct category of laser sources, characterized by an optimal balance among processing productivity, equipment cost, and the quality of the resulting structures. The pulse duration, measured in nanoseconds, is adequate for effective diamond ablation and reduces thermal damage to the processed surface [1]–[8].

A significant challenge in the laser processing of CVD diamonds involves establishing the correlation between the technological process parameters, such as pulse energy, number of pulses, and laser beam diameter, and the characteristics of the resulting structures, specifically the width and depth of the created cavities. Addressing this issue requires, among other steps, the development of models derived from experimental data. Nonetheless, the complex nature of the physical processes involved in laser processing of diamond considerably hinders the creation of adequately precise response surfaces. The application of artificial intelligence methods, particularly fuzzy logic, serves as an effective approach for modeling complex technological processes. Fuzzy models enable the formalization of expert knowledge through linguistic IF-THEN rules, which enhances model interpretability and accommodates qualitative patterns observed in experimental studies. Fuzzy systems exhibit significant robustness when handling incomplete data and possess the ability to generalize from limited training sets. This characteristic is particularly relevant for resource-intensive experiments that utilize costly materials. The application of fuzzy modeling to describe laser material processing has seen significant advancements in recent years [9]–[14].

The literature contains a limited number of studies that concentrate on the development of fuzzy models for nanosecond laser processing of polycrystalline CVD diamonds. As a result, a critical task involves the creation of a fuzzy model designed to predict the geometric parameters of the structures generated during the laser ablation of CVD diamonds, based on varying processing conditions. This work presents a study on the nanosecond laser processing of polycrystalline CVD diamonds. A fuzzy model was developed to predict the width and depth of the cavities formed, based on variables such as pulse energy, number of pulses, and laser beam diameter.

1 Experimental Study of Laser Processing of CVD Diamonds

This research utilized polycrystalline diamonds that were synthesized through microwave plasma chemical vapor deposition (CVD) in an acetylene atmosphere under reduced pressure [7]–[8].

Experimental studies were conducted on the laser processing of CVD diamonds using an LS-2134Y Nd:YAG laser. This system features electro-optical Q-switching and wavelength conversion from 1064 nm to 532 nm, with a pulse duration τ not exceeding 15 ns. The geometric parameters of the cavities were measured using a Model 130 profilometer (JSC PROTON Plant, Russia).

A face-centered central composite design for the experiment was constructed in the DesignXplorer module of ANSYS software to determine the values of three input parameters: *N* (number of pulses), *E* (pulse energy), and *D* (laser beam diameter) as detailed in Table 1.1. The width and depth of the laser-induced cavity in the CVD diamond (denoted as *S* and *H*, respectively) were taken as the output parameters.

Table 1.1 – Experimental design and results

N	*N* Number of pulses	*E* Pulse energy, mJ	*D* Beam diameter, μm	*S* Cavity width, μm	*H* Cavity depth, μm
1	2	15	800	240	14
2	1	15	800	280	21
3	3	15	800	260	18
4	2	17.5	800	330	39
5	2	20	800	450	44
6	2	15	600	260	21
7	2	15	1000	520	44
8	1	17.5	600	240	20
9	3	17.5	600	270	25
10	1	20	600	280	25
11	3	20	600	340	50
12	1	17.5	1000	300	23
13	3	17.5	1000	480	33
14	1	20	1000	320	24
15	3	20	1000	880	52

The acquired experimental data were compared with the findings of the research conducted by Mouhamadali et al. [5], which thoroughly examined the influence of nanosecond laser fluence (λ = 532 nm, τ = 40 ns) on the microstructure of CVD diamond. The comparison facilitates the interpretation of the physical nature of the observed effects, including the nonlinear growth of crater dimensions and the emergence of cracks. The difference between the current experiment and the study [5] is in the fluence range. In study [5], a fluence range of 4.9 to 50 J/cm² was considered, revealing that high-quality ablation free of cracks is achieved only at fluences above 35 J/cm². In the conducted experiment, with pulse energy E ranging from 15 to 20 mJ and spot diameter D ranging from 600 to 1000 μm, the computed fluence was around 1.9–7.1 J/cm². Thus, our research was performed within the value range designated by the authors of [5] as the “intense graphitization regime”.

It is worth noting that in experimental point No. 15 (see Table 1.1), at a maximum energy of 20 mJ and a spot diameter of 1000 µm, increasing the number of pulses from 1 to 3 resulted in a sharp increase in crater width from 320 to 880 µm. This effect is consistent with the conclusions of study [5] concerning phase transformations. The explanation is that the first pulse with low fluence primarily results in surface degradation rather than material removal, leading to the formation of a layer composed of graphite and amorphous carbon. Subsequent pulses then interact with this modified layer, inducing local overheating and extremely rapid material removal, which accounts for the abrupt increase in the diameter of the laser-induced cavity.

The morphology of the resulting cavities (see Figure 1.1) is defined by irregular edges, indicating that the thermomechanical mechanism of material removal predominates over sublimation.

Study [5] indicates that at the fluence levels employed in our experiment, the graphitization front progresses ahead of the ablation front, leading to the development of a substantial graphite layer. This induces stresses that cause macroscopic damage to the material, consistent with the observations in our experiment. Consequently, processing the material at low fluences leads to the formation of cracks within the graphitized layer, which propagate into the crystal bulk under thermoelastic stresses.

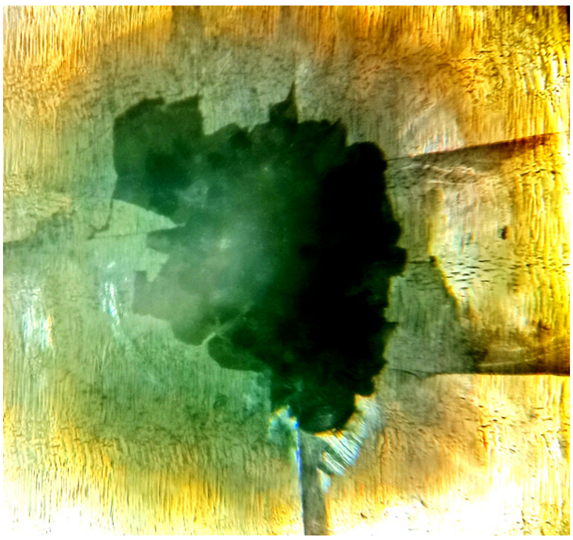

Figure 1.1 – Morphology of a laser-induced cavity in CVD diamond subjected to irradiation at a wavelength of 532 nm

Significantly, the results presented herein extend the findings of Mouhamadali et al. by incorporating an analysis of the laser beam diameter, a parameter not addressed in [5], which significantly impacts the geometry of the formed structures.

2 Determination of CVD Diamond Laser Processing Parameters Using a Fuzzy Model

Fuzzy modeling of the nanosecond laser processing of polycrystalline CVD diamonds was performed using the Mamdani fuzzy inference algorithm [9]. This algorithm was selected for its intuitive interpretability and its capability to formalize expert knowledge through linguistic rules. The model was implemented using the Scikit-Fuzzy library within the Python programming language.

The structure of the developed fuzzy system is presented in Figure 2.1. The system comprises three input parameters and two output parameters. The input parameters are *N* (number of pulses), *E* (pulse energy), and *D* (laser beam diameter). The output parameters are *S* (cavity width) and *H* (cavity depth).

The input parameters *N*, *E*, and *D* were represented by triangular membership functions, reflecting the discrete nature of the technological parameter variations observed in the experiment. The output parameters *S* and *H* were described by Gaussian membership functions, ensuring smooth variation of the output values and more accurate approximation of the experimental data (Figure 2.2).

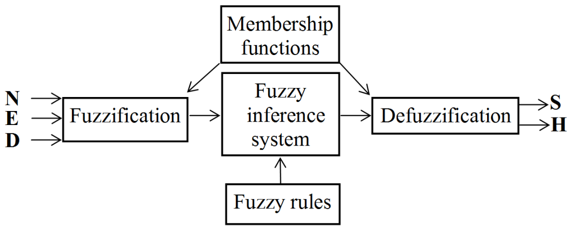

Figure 2.1 – Structure of the fuzzy system used for modeling the processing of polycrystalline CVD diamonds by a nanosecond laser

The following linguistic variables were defined for the input and output parameters.

For the input parameters, each variable was characterized by three terms: “low”, “medium”, “high”.

For the output parameters, each variable was characterized by nine terms: “tiny”, “very_low”, “low”, “med_low”, “medium”, “med_high”, “high”, “very_high”, “extreme”.

The extended set of terms for the output variables is due to the significant range of variation in the geometric parameters of the cavities and the need to describe nonlinear dependencies.

Two sets of rules were established to ascertain the output parameters *S* (cavity width) and *H* (cavity depth) based on the experimental data (Table 1.1).

The rule base for determining the cavity width (in the program code, the variables *N*, *E*, *D* correspond to the identifiers P1, P2, P3):

```
ctrl.Rule(P1['L'] & P3['L'], Width['low']),
ctrl.Rule(P1['L'] & P3['M'], Width['low']),
ctrl.Rule(P1['L'] & P3['H'], Width['med_low']),
ctrl.Rule(P1['M'] & P3['L'], Width['low']),
ctrl.Rule(P1['M'] & P3['M'] & P2['L'], Width['low']),
ctrl.Rule(P1['M'] & P3['M'] & P2['H'], Width['med_high']),
ctrl.Rule(P1['M'] & P3['H'], Width['high']),
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```
ctrl.Rule(P1['H'] & P3['L'], Width['low']),
ctrl.Rule(P1['H'] & P3['L'] & P2['H'], Width['medium']),
ctrl.Rule(P1['H'] & P3['M'], Width['low']),
ctrl.Rule(P1['H'] & P3['H'] & P2['M'], Width['high']),
ctrl.Rule(P1['H'] & P3['H'] & P2['H'], Width['extreme']),
ctrl.Rule(P2['H'] & P3['M'], Width['med_high']),
ctrl.Rule(P2['L'] & P3['M'], Width['low']),
ctrl.Rule(P1['L'] & P2['H'] & P3['H'], Width['med_low']),
```

The rule base for determining the cavity depth:

```
ctrl.Rule(P1['L'] & P2['L'], Depth['low']),
ctrl.Rule(P1['L'] & P2['M'], Depth['low']),
ctrl.Rule(P1['L'] & P2['H'], Depth['med_low']),
ctrl.Rule(P1['L'] & P3['H'], Depth['low']),
ctrl.Rule(P1['M'] & P2['L'] & P3['M'], Depth['tiny']),
ctrl.Rule(P1['M'] & P2['L'] & P3['L'], Depth['low']),
ctrl.Rule(P1['M'] & P2['L'] & P3['H'], Depth['high']),
ctrl.Rule(P1['M'] & P2['M'], Depth['med_high']),
ctrl.Rule(P1['M'] & P2['H'], Depth['high']),
ctrl.Rule(P1['H'] & P2['L'], Depth['very_low']),
ctrl.Rule(P1['H'] & P2['M'] & P3['L'], Depth['med_low']),
ctrl.Rule(P1['H'] & P2['M'] & P3['H'], Depth['medium']),
ctrl.Rule(P1['H'] & P2['H'], Depth['very_high']),
ctrl.Rule(P3['H'] & P2['L'] & P1['M'], Depth['high']),
ctrl.Rule(P3['L'] & P2['H'] & P1['H'], Depth['very_high']),
```

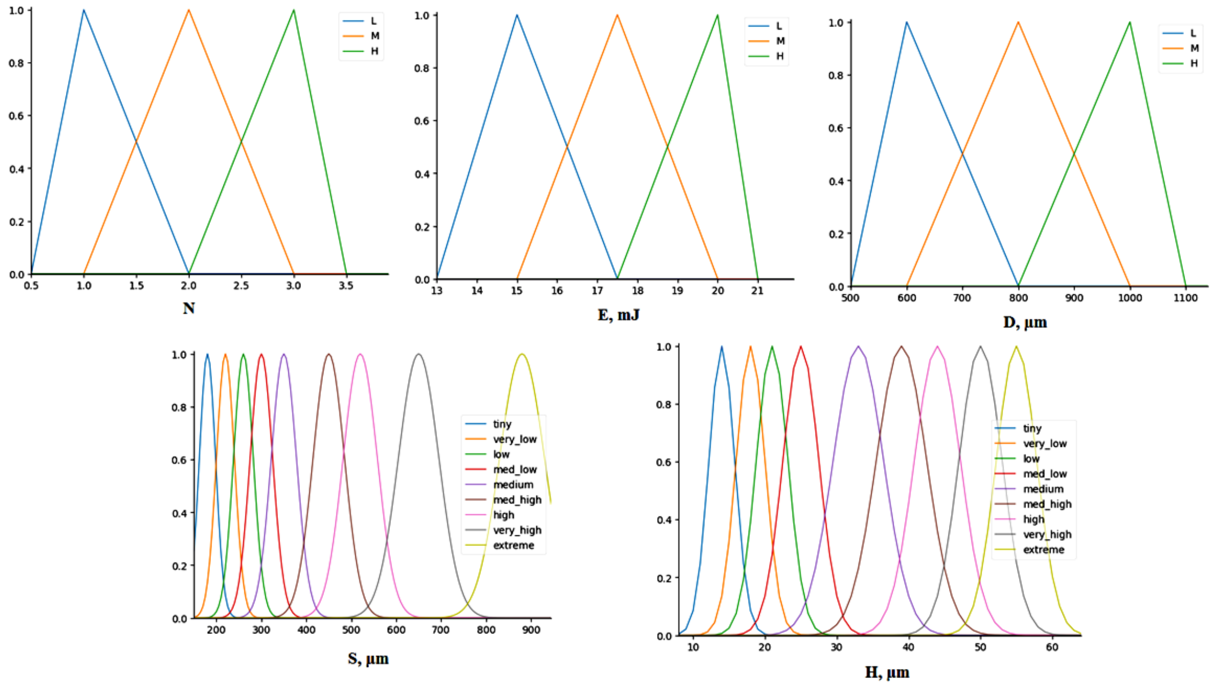

Figure 2.2 – Membership functions of the input and output linguistic variables

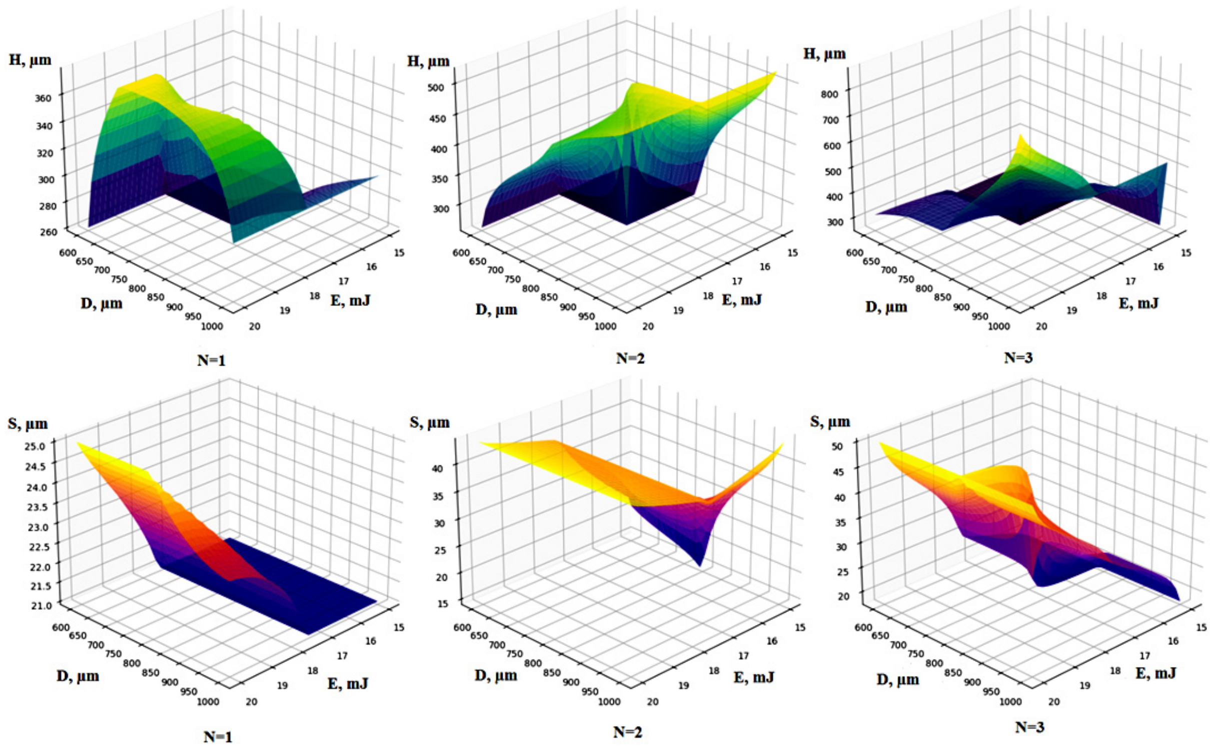

Figure 2.3 – Cavity depth H and width S as a function of processing parameters

Defuzzification was conducted to derive quantitative values for the output variables, thereby completing the fuzzy modeling process.

Figure 2.3 illustrates the relationship between the cavity depth H and width S in relation to the processing parameters, as derived from the fuzzy model.

The three-dimensional response surfaces (Figure 2.3), constructed for three values of the number of pulses ($N = 1, 2, 3$), show the relationship between pulse energy and beam diameter with respect to the geometric parameters of the cavity. The response surfaces exhibit a nonlinear character, thereby validating the application of fuzzy modelling to describe the process under study.

The quality of the fuzzy model was evaluated on a test data set (Table 2.1).

Table 2.1 – Test data set

N	*N* Number of pulses	*E* Pulse energy, mJ	*D* Beam diameter, µm	*S* Cavity width, µm	*H* Cavity depth, µm
1	1	16	900	310	26
2	1	18	800	240	24
3	2	17	700	245	30
4	2	19	600	285	38
5	3	16	700	240	17
6	3	18	900	500	38

The evaluation of the developed regression and neural network models was conducted using the following criteria:

Coefficient of determination

$$R^2 = 1 - \frac{\frac{1}{n}\sum_{i=1}^{n}(d_i - y_i)^2}{\frac{1}{n}\sum_{i=1}^{n}(d_i - \bar{d})^2}.$$

Mean Absolute Error (MAE)

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|d_i - y_i|.$$

Root Mean Square Error (RMSE)

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(d_i - y_i)^2}.$$

Mean Absolute Percentage Error (MAPE)

$$MAPE = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{d_i - y_i}{d_i}\right| \cdot 100,$$

where d_i represents the values determined experimentally, y_i denotes the values derived from the fuzzy model.

The results of the fuzzy model evaluation are provided in Table 2.2.

Table 2.2 – Fuzzy model evaluation results

Criterion	Central composite design dataset		Test dataset	
	S	*H*	*S*	*H*
RMSE	34.3 µm	0.8 µm	41.6 µm	3.5 µm
MAE	20.2 µm	0.4 µm	33.0 µm	3.0 µm
MAPE	6.2%	1.4%	12.2%	12.3%
R^2	0.9552	0.9956	0.7940	0.7906

The analysis of the obtained metrics indicates a high adequacy of the constructed model. In the training dataset, the coefficient of determination for cavity depth attained $R^2 = 0.9956$, indicating an almost perfect correspondence between the model predictions and the experimental data. The coefficient of determination for cavity width is also high, amounting to $R^2 = 0.9552$. The mean absolute percentage error for the training dataset does not exceed 6.2% for width and 1.4% for depth, demonstrating accurate approximation of the experimental dependencies.

On the test dataset, the model demonstrates satisfactory generalization capability. The comparison of the metrics from both the training and test datasets allows for an assessment of the model's generalization ability. The coefficient of determination is observed to decrease to 0.7940 for width and to 0.7906 for depth when moving from the training dataset to the test dataset, signifying a moderate decline in accuracy with fresh data. The MAPE values for the test dataset (12.2% and 12.3%) exceed the corresponding values for the training dataset, suggesting a degree of model overfitting; yet, the absolute error values remain within acceptable limits for technological forecasting tasks. The compactness of the rule base (15 rules per output parameter) demonstrates efficient utilization of experimental data in model construction. Moreover, the obtained accuracy metrics indicate that the model adequately captures the main regularities of the process under study.

Conclusion

This study presents a comprehensive examination of the nanosecond laser processing of polycrystalline CVD diamonds using a Nd:YAG laser ($\lambda = 532$ nm, $\tau \leq 15$ ns). Additionally, a fuzzy model was created to predict the geometric parameters of the resulting structures. The analysis indicated that, given the specified processing parameters, the process operates within the intense graphitization regime. This leads to nonlinear dependencies and the development of cavities with irregular edges, attributed to the dominance of the thermomechanical material removal mechanism. A fuzzy model employing the Mamdani algorithm was created, incorporating three input parameters (number of pulses, pulse energy, beam diameter) and two output parameters (cavity width and depth). The fuzzy model, comprising 15 rules for each output parameter, exhibited a reasonably high accuracy in approximating the experimental data. The results obtained validate the effectiveness of applying fuzzy logic for modeling laser processing of CVD diamonds and can be used to optimize the technological regimes for nanosecond laser ablation of polycrystalline diamond materials.

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