Fourier Analysis with Gini Coefficient: A New Approach to Assess Surface Topography in Direct Laser Interference Patterning

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Direct Laser Interference Patterning (DLIP) is an emerging manufacturing technology for creating functional surfaces. To integrate DLIP into industrial processes, reliable and rapid methods for determining the quality of the produced microstructures are essential. Surface roughness evaluation methods are typically designed to quantify variations in surface morphology relative to an ideal uniform surface. As a result, these methods are inadequate for assessing the quality of periodic structures generated by DLIP, requiring the implementation of additional algorithms to mitigate their influence. Recently, a method that uses Gini analysis on surface topographical parameters was established for this purpose. It first divides the surface into a series of decomposed parts according to the period and then uses the Gini coefficient to statistically describe the roughness parameters obtained from each part to evaluate the homogeneity. However, the resulting value is strongly dependent on the type and number of parameters selected. This work introduces a novel approach that employs Gini analysis of two-dimensional Fast Fourier Transform (2D FFT) on topography images, providing both qualitative and quantitative assessments of texture homogeneity. The comparison of those two methods indicates that the FFT Gini method correlates well with homogeneity measurements directly taken from the surface topography and demonstrates the advantage of evaluating the structuring process at high proceeding speed.
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1. Introduction

Periodic structures are crucial in numerous scientific and industrial applications because of their capability to replicate natural phenomena and achieve precise surface functionalities. For instance, the iridescence of butterfly wings [1], the self-cleaning capability of lotus leaves [2], and the structural coloration of peacock feathers are all outcomes of surfaces having periodic patterns [3].

Among the processes that can be used for producing periodical surface structures, Direct Laser Interference Patterning (DLIP) stands out due to its compatibility with industrial processes and its ability to treat large areas in a one-step [4-6]. The DLIP technique employs the superposition of multiple coherent laser beams, which form a periodic distribution of the laser intensity on the material surface, a phenomenon known as interference [7]. This technology has already been implemented on different materials, leading to the improvement of several functions, such as biocompatibility, wettability, and light management [8-11].

In order to facilitate the integration of DLIP into industrial processes, it is essential to develop reliable and rapid methods for determining the quality of the produced microstructures. Parameters used in evaluating load-bearing components, such as the Abbott-Firestone curve or bearing area curve, provide crucial information regarding surface functionality, particularly in terms of wear resistance. However, these parameters cannot be used to describe the homogeneity of periodic patterns. Traditional methods for evaluating the surface quality, such as Root Mean Square (RMS) roughness [12] or average height (or depth), are suitable for quantifying the average variations in the amplitude of the surface heights. However, these methods are also not capable of describing the quality of repetitive structures. Other approaches that incorporate machine learning algorithms have demonstrated considerable potential in recognizing and assessing more intricate and subtle surface textures [13-14]. However, they typically require extensive training datasets to achieve optimal performance and are often computationally intensive, which may restrict their implementation in industrial applications that prioritize simplicity and speed. Thus, alternative methods are required to assess the surface homogeneity of periodical or quasi-periodic structures.

A recent method proposed by Lechthaler et al. has been implemented to evaluate the quality of repetitive structures [15]. The method involves dividing a surface topography image into segments based on the texture period and using the Gini coefficient to statistically describe the roughness parameters variation between the segments. Then, the data obtained for all segments is compared, determining the Gini coefficient of the structure [16]. While surfaces having a Gini coefficient of 1 are perfectly periodic, a value of 0 means perfectly flat. However, the resulting value is significantly influenced by the type of roughness parameters selected. For instance, the value calculated based on height parameters differs from those obtained by analyzing other statistical parameters, such as kurtosis, Sk. Consequently, the value of the Gini coefficient is only useful for comparison between different experiments when the exact same set of parameters is used.

Other analytical approaches, such as those based on the two-dimensional Fast Fourier Transform (2D FFT), allow for a comprehensive analysis of surface textures by converting the surface profile into its frequency components [17]. This technique enables the identification of periodic structures and their irregularities. The primary features of the periodical surface structure are captured in the first-order peak of the FFT, as detailed in [18–20]. By analyzing the intensity distribution of this first FFT order, the quality of the periodical structure can be evaluated.

This approach of analyzing the quality of fabricated periodic structures in the Fourier space can be implemented in scatterometry. Soldera et al. and Schröder et al. have demonstrated an optical system based on scatterometry that directly provides the FFT spectrum of DLIP patterned surfaces, allowing for the identification of structure depth and periodicity [21-22]. However, a method for assessing the pattern quality with this optical system has not yet been developed. Therefore, analytical approaches based on the FFT spectrum of the surface topography have the potential to be applied in this optical system to obtain more detailed characteristics of the analyzed surface topography.

This study introduces a novel analytical approach that uses the Gini coefficient to analyze the first-order peak in 2D FFT of periodical structure structures. Correlations between surface topography and homogeneity quantification by Gini analysis are established and discussed in relation to the laser repetition rate. A comparison is made between the proposed method and the established surface roughness Gini method, demonstrating a possible implementation in the future for high-speed surface analysis.

2. Materials and methods

2.1 Materials

The laser patterning experiments were performed on 0.75 mm thick stainless steel plates (1.4301). The initial surface roughness (Sq) of the untreated substrates was 0.59 µm. Prior to structuring, the samples were cleaned with ethanol to eliminate any surface contaminants.

2.2 DLIP structuring setup and surface characterization

Figure 1 illustrates the experimental setup used in the experiments. The study employs a picosecond-pulsed solid-state laser (Edgewave PX200, Germany) with a 30 W output power, operating at a wavelength of 1064 nm and a pulse duration of 12 ps. The laser's repetition rate is adjustable from 1 to 30 kHz. An innovative DLIP module called Extended Laser Interference Patterning System (ELIPSYS®, SurFunction GmbH) was used in this work, which enables fast and cost-effective fabrication of periodic surface structures [23]. This configuration generates an elliptical-shaped spot with a periodic line-like interference pattern covering an area of 870 µm by 126 µm, as illustrated in Figure 1b. The spatial period of the interference pattern was 5.9 µm. The microstructuring of samples was conducted in air at atmospheric pressure.

The metal samples were mounted on an XY moving stage (Aerotech, Inc., Pittsburgh, USA), which enabled the positioning to be carried out with a maximum travel distance of 500 mm and a maximum speed of 500 m/s. During the laser structuring process, the samples were moved in the direction parallel to the interference lines (perpendicular to the spot's long axis). The distance between two consecutive pulses in the y-direction is referred to as the pulse-to-pulse distance (Pd), as illustrated in Figure 1. Each test was conducted by varying the laser repetition rate (f_R) from 1 to 30 kHz, and the Pd from 0.8 to 10 µm, resulting in spot overlaps (OV) ranging from 92.1 to 99.4 %, which is defined by Equation 1:

$$OV = 100\left(1 - \frac{P_d}{d}\right). \quad (1)$$

The topography of the structured samples was determined using an optical confocal microscope (Sensofar S Neox 3D, Surface profiler, Barcelona, Spain) with a 50x objective. The microscope provided lateral and vertical resolutions of 170 nm and 3 nm, respectively.

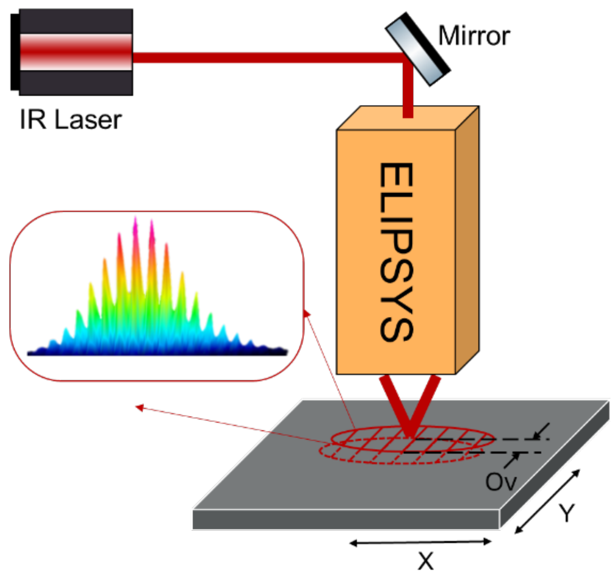

Fig. 1 A graphical representation of the novel ELIPSYS module, which employs the Direct Laser Interference Patterning (DLIP) technique with a detailed illustration of the laser spot, which features an elongated shape with a periodic intensity profile.

2.3 Homogeneity analysis of the fabricated structures

The homogeneity of the measured topographies was quantitatively assessed using an algorithm that implements the Gini analysis of the Fourier space. The algorithm was implemented in Python with the support of the libraries OpenCV [24] and is outlined in the flowchart in Figure 2a. To demonstrate the working principle of the algorithm, an image generated by a Python script that calculates the sinusoidal 2d profile was used (see Figure 2b). The algorithm consists of four main steps:

I. Fourier transform: Initially, a 2D FFT is applied to the surface topography data (Figure 2b) to retrieve the frequency spectrum that is presented in Figure 2c. This transformation is of crucial importance as it converts the spatial distribution of the surface structures into the frequency domain. Thus, the identification and analysis of periodic patterns and their spatial frequencies is possible.

II. Extraction of the profile of the first FFT order peak: the first FFT order corresponds to the primary spatial frequency that represents the DLIP-induced texture. Owing to the inherent symmetry in the FFT space, it is enough to analyze only one of the two first orders. In this case, a horizontal profile of the +1st diffraction order is extracted for further analysis, as indicated in Figure 2c.

III. Calculation of the Lorenz curve [25]: the Lorenz curve from the extracted profile of the first-order peak of FFT is calculated. In Figure 2e, the Lorenz curve is plotted as a function of the cumulative share of spatial frequencies to the cumulative intensity of the first FFT order profile. A unique representation of the Lorenz curve, also known as the line of equality, symbolizes the hypothetical scenario of ideal uniform distribution [26]. In Figure 2e, the line of equality is plotted as a red dotted line, illustrating the contrast between the calculated (blue solid line) and perfect equal distribution.

IV. Gini coefficient calculation: the Gini coefficient for the intensity distribution of the extracted profile is calculated. The Gini coefficient, also known as the Gini index, is a measure of inequality based on the Lorenz curve of a specific distribution [27]. The Gini coefficient, denoted as G, is given by Equation 2:

$$G=\frac{A}{A+B}, \tag{2}$$

where A represents the area between the line of equality (or the 45-degree line) and the Lorenz curve of the investigated distribution; B represents the area under the Lorenz curve, which highlights the cumulative share of income or wealth up to a certain percentage of the population.

The value of G ranges from 0 to 1. In economic terms, a value of 0 represents perfect equality, whereby all individuals possess identical income or wealth, corresponding to a completely flat Lorenz curve with no peaks. Conversely, a value of 1 indicates the maximum degree of inequality, whereby a single individual possesses all the income or wealth, as illustrated by a Lorenz curve with a single, infinitely sharp peak.

In this study, the Gini coefficient is employed as a measure of the variability in the intensity of spatial frequencies obtained through FFT. A value approaching 1 indicates that the intensity distribution in the primary FFT peak is concentrated around a single spatial frequency, which indicates a highly regular and homogeneous periodic texture. In contrast, lower Gini values indicate a more dispersed intensity distribution, which corresponds to less uniform and more irregular structures. To sum up, a Gini coefficient approaching unity indicates a high degree of uniformity and periodicity in the structure.

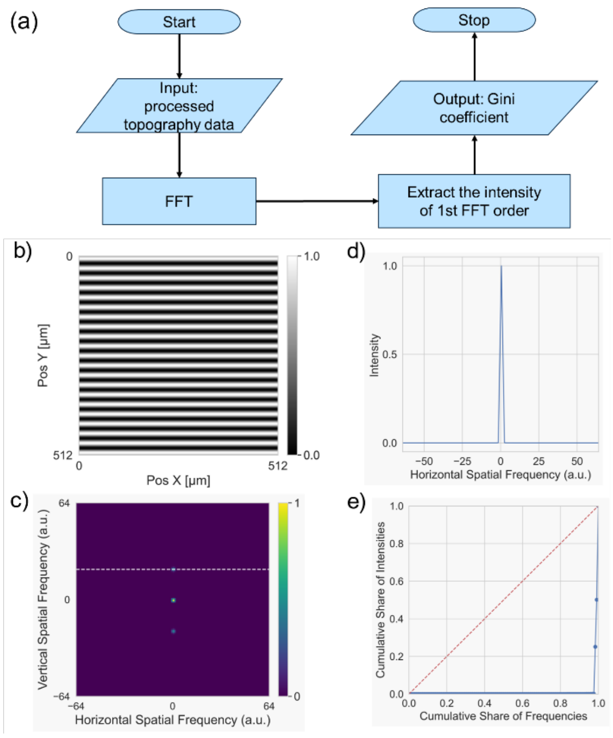

Fig.2 (a) The flowchart illustrates the implementation of Gini analysis on a 2D FFT of the surface topography using Python script, accompanied by sample output images generated during code execution: (b) Surface topography; (c) FFT spectrum of the surface topography; (d) Extracted intensity profile of the +1st FFT order; (e) Lorenz curve of the extracted intensity profile.

3. Results and discussion

3.1 Topography of DLIP-treated stainless steel

Firstly, the steel samples were structured according to the procedures described in Section 2.2. A comparative study was conducted across a range of overlaps and repetition rates. The following combinations were considered: low pulse overlap (92.1%, 96.0%), high pulse overlap (99.2%, and 99.4%), low repetition rate (1 kHz, 5kHz, 10 kHz), and high repetition rate (20 kHz, 30 kHz). To gain further insight into the surface structures, selected samples were examined using a confocal microscope.

Figure 3 shows the selected surface morphologies obtained from the DLIP process, representing the surface quality typically achieved under four conditions: (a) low pulse overlap with low repetition rate; (b) high pulse overlap with low repetition rate; (c) low pulse overlap with high repetition rate, and (d) high pulse overlap with high repetition rate. The used process parameters are indicated in the figure caption.

The topography of the first three conditions features well-defined regularity and homogeneity of the fabricated periodic strictures, as demonstrated in Figures 3a, 3b, and 3c. However, the topography in the condition with both high pulse overlap and high repetition rate (Figure 3d) exhibits noticeable waviness and depth variations of the periodical lines. To quantitatively evaluate the structure quality, we applied an already established method from the literature (as described in the introduction section) that employs the Gini coefficient directly on the structure topography, which we refer to as “Topography Gini” in the following sections [13].

The results showed that the quality of the DLIP structure depicted in Figure 3a, which was fabricated with a low pulse overlap and with a low repetition rate, was not reduced either with an increase of pulse overlap (Figure 3b) or the laser repetition rate (Figure 3c). This is evidenced by the "Topography Gini" values of 0.859, 0.860, and 0.869, respectively. However, when both the laser repetition rate and the pulse overlap were simultaneously increased, as shown in Figure 3d (99.2 % overlap and 30 kHz), the result of the "Topography Gini" value decreased to 0.686. This decrease can be quantified as a reflection of the reduction in the quality of the periodical pattern.

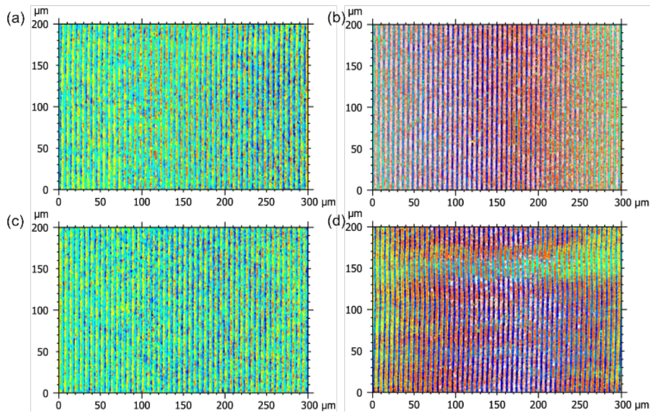

Fig. 3 Confocal images of DLIP processed surfaces with a), c) 96 %, and b), d) 99.2 % pulse-to-pulse overlap at a repetition rate of a), c) 1 kHz, and b), d) 30 kHz.

3.2 Analysis of DLIP-treated surfaces in the Fourier space

A quantitative assessment of the surface quality of the treated stainless-steel surfaces was conducted using the proposed method based on Gini analysis in the Fourier space (detailed in Section 2.3). Examples of the resulting outputs based on the DLIP patterns from Figures 3b and 3d are illustrated in Figure 4.

The sharp peaks in the FFT image shown in Figure 4a can be directly correlated to a highly regular and coherent spatial frequency (as simulated in Figure 2c). Moreover, the first-order peak profile exhibits a slender shape, and a few high-intensity values can be observed at the center position (Figure 4b). In contrast, the FFT spectrum (Figure 4c) from the topography in Figure 3d demonstrates a broad spread of intensity across all orders in the horizontal direction. This is clearly visible in the extracted horizontal profile of the first intensity order in Figure 4d.

These results suggest that within the tested parameter range, the laser parameters significantly affect the surface morphology, which strongly affects the intensity and shape of the profiles extracted from the first-order FFT signal. Therefore, the shape of the distribution of the intensity profiles shows a priori that it could be used as a preliminary indicator of the surface quality.

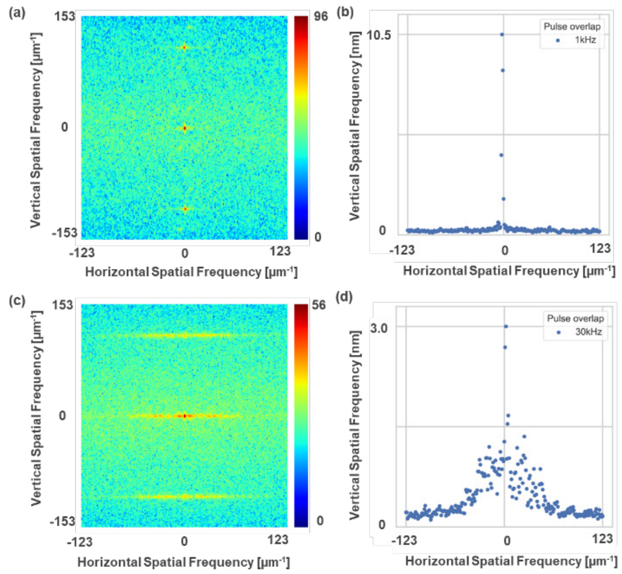

Fig. 4 Characterization of DLIP surface topographies obtained through confocal microscopy and their corresponding two-dimensional fast Fourier transform (2D-FFT) analysis and profiles extracted from the first order at pulse-to-pulse overlap of 99.2% with different repetition rates: (a, b) 1 kHz, (c, d) 30 kHz.

3.3 Comparison between Gini analysis on the FFT Spectrum and directly on the topography

The proposed method in this study, referred to as "FFT Gini", was employed to indirectly describe the homogeneity of a periodic line-like structure from the analysis of the first order from the topography 2D FFT (section 3.2). In contrast, the "Topography Gini" describes the homogeneity directly from the surface topography. Thus, to validate the here presented approach, both methodologies were compared. In the case of the "Topography Gini" analysis, roughness parameters for mean structure height were selected (as in [16]).

Figure 5 presents a series of Gini coefficient values obtained from these two approaches, considering the surface structures created by DLIP, with pulse overlap of 99.2% and 99.4% and varying repetition rates from 1 kHz to 30 kHz. The plot includes a linear regression fit, which indicates the 95% confidence interval. Despite the differences in the absolute values acquired from these two methods, a similar declining trend can be observed with the increased laser repetition rate as well as for low pulse overlaps. The correlation between these two methods was analyzed using Spearman's correlation coefficient, r h o rho, which is a measure of the strength and direction of association between two variables [29]. This value ranges from -1 to +1, indicating strong negative and positive association. The results indicate a strong positive correlation between the two values obtained from these two methods, with a Spearman's rho value of 0.67 and a p-value of 0.001(less than 0.05), thereby confirming that this effect is also statistically significant. This indicates that the two measures provide similar results in general. Therefore, the values calculated from the "FFT Gini" method can be regarded as a quantitative measure of the changes in surface quality.

On the other side, compared to the values obtained from the "Topography Gini" method, the "FFT Gini" values exhibited higher sensitivity to the increased frequency under high pulse conditions (pulse overlap 99.2% and 99.4%), which is reflected by a steeper slope of the regression fit (purple and red dashed lines in Figure 5). This observation is confirmed by a regression analysis [28] based on all the investigated experimental conditions, where the homogeneity values calculated from both methods were fitted as a function of pulse overlap, laser repetition rate, and their interaction, which is the combined influence of these two variables. The standardized coefficient and corresponding p-values obtained from each regression analysis are displayed in Table 1.

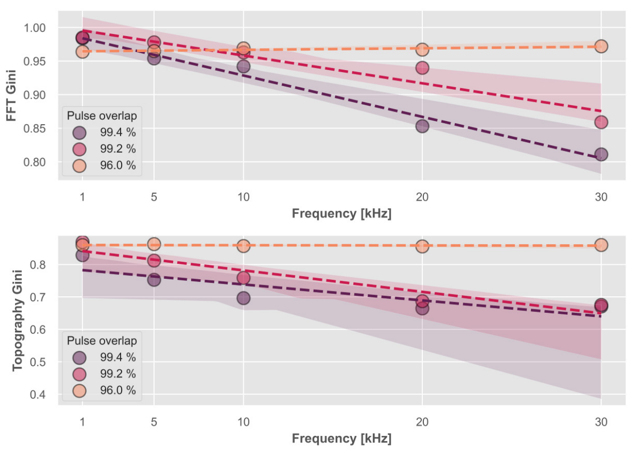

Fig. 5 Comparison of homogeneity evaluation methods of the DLIP structured steel surfaces fabricated with varying repetition rates and overlaps (OV).

Table 1 Results from linear regression analysis

	Standardized Coefficient	P Value
FFT Gini		
Repetition Rate	0.326	0.04*
Pulse Overlap	-0.515	0.00*
Repetition rate ×Pulse Overlap	0.415	0.01*
Topography Gini		
Repetition Rate	0.548	0.00*
Pulse Overlap	-0.508	0.00*
Repetition rate ×Pulse Overlap	0.342	0.01*

* P-value < 0.05 indicating statistical significance [30]

The results demonstrated a significant impact of both laser repetition rate and pulse overlap on the two Gini values. The "Topography Gini" value exhibited a more pronounced correlation with the repetition rate, as evidenced by a standardized regression coefficient of 0.548 in comparison to 0.326 obtained from the "FFT Gini" value. The effect of pulse overlap was comparable for the two Gini values, as indicated by regression coefficients of -0.515 and -0.508, respectively. In contrast, the combined influence of repetition rate and pulse overlap is more strongly associated with the FFT Gini (coefficient 0.415) than with the topography Gini (coefficient 0.342). This suggests that the FFT Gini is more responsive to changes in the interaction of the two parameters. Therefore, the “Topography Gini” can be applied to more general processes, while “FFT Gini” is suitable for the evaluation of processes with both high pulse overlaps and high repetition rates.

4. Conclusion

This study demonstrates that the proposed analytical method (“FFT Gini”), which employs Gini analysis on the FFT spectrum from fabricated structure topographies, is an effective way of determining the quality of periodic structures. The influence of laser parameters, including pulse overlap and repetition rate, on surface homogeneity was investigated. The results of both methods indicate that an increase in the laser repetition rate negatively impacts structure homogeneity, particularly at high pulse overlaps (> 99%). However, for overlaps below 99%, variations in repetition rate have a minimal effect on structure depth and homogeneity. This indicates that lower overlaps can maintain quality while enabling faster processing speeds.

The correlations between “FFT Gini” and “topography Gini” were discussed in relation to the laser repetition rate, pulse overlap, and their combined effect on the line-like DLIP structures. The result indicates that both methods generally yield similar results, with the “FFT Gini” being particularly advantageous for processes with both, high pulse overlaps and high repetition rates.

It is important to note that other process parameters, such as laser fluence and spot size, affect the final structure homogeneity, even though they were not investigated in this paper. Moreover, the exact threshold of the Gini coefficient that is used to differentiate between high- and low-quality processing should be correlated with the specific functional requirements for the intended application in each use case. The method is versatile and can be applied to surfaces of different materials, as it analyses surface topography independently of the material on which it was fabricated. Therefore, the Gini method can be effectively applied as long as the measurement device can clearly capture the structure's topography.

However, this approach does have certain limitations. It is currently designed to analyze the spatial frequency distribution along a one-dimensional cross-section of the initial FFT order, which constrains its ability to capture the full spectrum of spatial frequencies associated with potential inhomogeneities. As a result, spatial frequencies that deviate from the main peak in FFT, which nevertheless contribute to the DLIP structures as inhomogeneities, are not considered. To comprehensively account for all potential inhomogeneities across a range of spatial frequencies, a two-dimensional Gini analysis is required.

In summary, this method can provide both quantitative and qualitative evaluation of the surface quality from the Fourier spectrum of the fabricated pattern topography, which can potentially be implemented in the direct monitoring of the surface using the FFT optical system proposed by Soldera et al. and Schröder et al. [21-22]. To enhance the robustness of the method in detecting inhomogeneities across the entire frequency spectrum, a 2D Gini analysis must be implemented.

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