Relative positioning method for near-field beam spot array with optical microscope image of lithographic patterns using linear regression

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A method for simply analyzing the relation between spot positions of near-field beam sources with micrometer pitch is proposed using an optical microscope. Based on the locations of spots in an optical microscopy image of lithographic patterns, the effective relative position is derived using simple linear regression. Numerical analysis is performed to introduce the concept and to evaluate the methodology with random noise. The accuracy and uncertainty of the proposed method are discussed. To confirm the method’s feasibility, the experiments are conducted using fabricated probe array, and the experimental and numerical results are compared on the basis of uncertainty. An arbitrary pattern is recorded with respect to relative coordinates obtained based on the effective positions. We suggest a simple strategy for controlling beam spot array locations for pattern design in near-field lithography with less than 5-nm uncertainty.

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1. INTRODUCTION

In order to overcome the diffraction limit, the near-field concept has attracted intensive attention for allowing high resolving power to nanotechnology. Nanometric structures such as antennae, apertures, and grooves with subwavelength geometries generate evanescent electromagnetic waves, which have been widely studied and exploited in the application of near-field optical techniques for high spatial-resolution measurement and fabrication [1,2]. At visible wavelengths, the light spot transmitted through a small aperture in an opaque metal screen is locally confined and exponentially attenuated perpendicular to the exit surface in the near-field regime. However, the near field has intrinsic difficulties under conditions of low output power and a restricted operation range from the source. Combined with the surface plasmon effect, the light transmission can be highly enhanced by the ridge shape of the nanoaperture [3,4].

A near-field scanning optical microscope (NSOM) has been developed in recent decades with metallic tip scanning along the sample of interest, performing imaging through interaction of the electromagnetic field with the nanostructures and, hence, providing super-resolution capabilities [5,6]. In addition, near-field scanning probe lithography has been reported as an alternative lithographic technique that can generate nanoscale pattern structures simply, using optical near-field spot with resolution beyond the diffraction limit. However, as those near-field techniques are intrinsically based on the serial process employed by the scanning probe, they suffer from low throughput, which leads to advanced fashioning of a parallel regime with a two-dimensional probe array structure. The multiple optical sources from the probe array can induce a large number of subwavelength beam spots in the near field. These beam spots can be simultaneously operated in separated multiple areas with their own registration [7–9].

In lithographic application, each location of the various individual patterns transferred onto the photoactive material over a large area is highly dependent on the primitive position of the near-field beam spot on the probe. Position errors in the spot locations can induce stitching issues throughout the whole patterning area and have an effect on the pattern design and quality across the border between each field. Therefore, it is important to obtain the position values relative to each other for near-field beam spots in a probe array. We can expect that their variation is primarily due to device fabrication uncertainties. Typically, the entire body of a polynomial-shaped probe tip is constructed via a microelectromechanical (MEMS) fabrication process with microscale tolerance, with nanoapertures being perforated on the end of the tip using a focused ion beam...
near field emerging from a single nanostructure [10]. These studies have focused on mapping the subwavelength light fields for expecting the spatial distribution of intensity in detail with a high-resolution imaging process. However, it seems that it is difficult to simultaneously measure an extended arrangement of near-field sources with micrometer pitch and determine their geometrical correlations at once. Moreover, the approach to detecting the beam spot intensity distribution could be sensitive to circumstantial noise factors, and a series of microscopic optics could additionally accumulate the errors to outcomes, especially affecting geometrical information. Pixel size of a charged coupled device (CCD) camera is also critical to the capability of measuring characteristics of beam spots, as sub-pixel accuracy is required [14]. In order to manage multiple near-field sources efficiently, with respect to each other and within a nanoscale margin, the position system of sources need to be analyzed to design the improved performance for all units of probe array in application.

In this study, we propose a practical method of relative position analysis for near-field beam spots in an optical contact probe array with lithographic technical support. When light is projected to photoresist (PR), optical distribution is transferred and revealed as a nanostructure pattern with geometrical parameters. The pitches of all beam spots are not exactly identical and can differ from the desired parameters, depending on the tolerance of the fabrication process. For near-field lithography in particular, the relative deviations in the beam spot locations is required to be known, so that the target pattern can be designed appropriately across the required area with no stitching errors. The location errors of beam spot and nanoapertures are also transferred to the exposed patterns. Hence, if we obtain the position values of spot patterns and evaluate them with respect to each other, the entire coordinate system could be controlled to facilitate the production of large-area patterns through extended regions.

Therefore, we introduce a methodological concept for deducing the effective positions of near-field beam spots from an optical microscopy image, and discuss the feasibility of this fast and simple method, considering the accuracy and uncertainty. Numerical analysis is conducted to determine the effective relative position (ERP), and uncertainties calculated with random noise are compared with those obtained via experiment. Furthermore, we demonstrate the production of multi-area patterns using a near-field beam array depending on the relative optimal coordinates determined based on the ERPs.

2. METHODOLOGICAL CONCEPT

Near-field beam spots are generated by nanoapertures at the ends of an optical probe array. The field distribution can be visualized as certain shaped features in photoactive materials using a lithographic technique. All of the produced patterns reflect the characteristics of each beam spot, such as its shape, intensity, and dimensions. We assume that each nanoaperture on the optical probes creates an \( N \times N \) array of spot patterns, with sizes ranging from tens to hundreds of nanometers. After the development process, patterns on the substrate were captured as an image by an optical microscope. Thus, for practicality, we consider an experimental condition with use of a conventional optical microscope with a high numerical-aperture (NA) objective lens of 100× magnification. Equipped microscopy camera allows the captured image to be divided by discrete unit pixels, so that the output image becomes a good indicator of the registration of each spot pattern location by imaginary coordinates within a defined field of view. We assumed that each spot pattern size is sufficiently larger than a resolution of the object lens in an optical microscope. Since an isolated spot pattern in a detected image occupies an arbitrary region comprised of several pixels enough to be qualified by Nyquist’s theorem, a spot pattern location can be assigned as a point depending on the diffracted distribution for position analysis. Thus, each location of a spot pattern is determined by identifying the intersection point of vertical and horizontal lines fitted with intermediate values defined by the edge values of left-right and up-down sides in shape distribution of the spot pattern.

A schematic view of the background condition for obtaining the position of each beam spot by optical probe array is described in Fig. 1. Spot array pattern locations form an \( N \times N \) square matrix with \( (x_{ij}, y_{ij}) \) coordinates. By analyzing the position matrix for each group of spot patterns, we can define the ERP for each probe as a representative point. Note that any point in the spot pattern matrix can be selected as the ERP, which is assigned coordinates \((a, b)\). Then, if we determine the target location of ERP, all other spot pattern locations in the matrix can be identified relative to \((a, b)\). Figure 2 shows detailed descriptions of the parameters used to construct an expression for each spot pattern. In the coordinate system of the captured image, the counterclockwise direction is assumed to be positive for an angle \( \theta \), and the first pixel is set as the origin. The ERP is selected as a center point of the matrix.

![Fig. 1. Schematic diagram of background condition to illustrate methodological concept. \( N \times N \) arrays of spot patterns are obtained by \( 2 \times 2 \) optical probe array and captured by an optical microscope. An imaginary coordinate system is constructed and an ERP \((a_k, b_k)\) is defined for each probe. \( k \) is the probe number.](image-url)
The correlations between the spot-pattern positions are specified with respect to \((a, b)\) coordinates.

A \(5 \times 5\) spot pattern array \((N = 5)\) is assumed in order to introduce the required expressions. The general form of \(x_{ij}(i = \text{row}, j = \text{column})\) for each \(x\)-axis position can be expressed as

\[
x_{ij} = a_{ij}d \cos \theta + b_{ij}d \sin \theta + a,
\]

where \(d\), \(\theta\), and \(a\) denote the relative displacement between the spot patterns, the rotation angle relative to the axis, and the \(x\)-axis ERP, respectively. \(a_{ij}\) and \(b_{ij}\) are varied coefficients depending on \(x_{ij}\).

Because \(\theta\) is far less than 1, all terms are subjected to small-angle approximation to simplify the equations. Thus,

\[
x_{ij} = a_{ij}d \left(1 - \frac{\theta^2}{2}\right) + b_{ij}d \theta + a,
\]

\[
\text{for } \cos \theta \approx 1 - \frac{\theta^2}{2} \text{ and } \sin \theta \approx \theta.
\]

In the above equations, coefficients \(a\) and \(b\) can be estimated as ERP values through regression analysis with all \(x_{ij}\) and \(y_{ij}\) values. However, these equations contain three variables; thus, a surface-fitting process is required in order to find the values of the coefficients. This process is very complex and is easily affected by statistical errors. Therefore, we select the central point of the matrix as the optimal target point for ERP, depending on the symmetrical coefficients of \(\cos \theta\) in the expressions. The summation of the two coupled equations can eliminate the cosine terms of \(d \theta^2\), and all equations can be reduced to linear equations for superposed position \(X_n\) or \(Y_n\). Hence, the general form for \(X_n\) is

\[
X_n = x_{ij} + x_{ij'}
\]

\[(2.1)\]

where \(x_{ij}\) and \(x_{ij'}\) are the pair of spot pattern positions conjugate to each other with respect to \(\cos \theta\) term in matrix. Subscript \(n\) denotes the calculated sampling order for superposition. From the Eq. (1.1), \(X_n\) can be expressed as

\[
X_n = (a_{ij} + a_{ij'})d \cos \theta + (b_{ij} + b_{ij'})d \sin \theta + 2a.
\]

By \(a_{ij} + a_{ij'} = 0\) and small-angle approximation, governing correlation for the matrix can be derived as

\[
X_n = d \theta y_{X_n} + 2a,
\]

\[(2.3)\]

where \(X_n\) and \(y_{X_n}\) are main variables to obtain \(a\) in ERP. \(X_n\) is calculated from position data of spot patterns and \(y_{X_n}\) is derived by both of \(b_{ij}\) and \(b_{ij'}\) determined by configuration of matrix. \(x_{ij}\) values of the central column \((i = \frac{N+1}{2})\) in the matrix have no sinusoidal terms for subtraction so that they are superposed based on \(i' = i\). \(j' = (N + 1) - j\). The value of \(x_{ij}(i = \frac{N+1}{2}, j = \frac{N+1}{2})\) has no pair, then is multiplied by two for an expression of \(X_n\).

Finally, \(a\) and \(b\) in ERP are simply expected based on linear regression analysis for \(y_{X_n}, X_n\) and \(y_{Y_n}, Y_n\).

Each \((a_{sb}, b_{sb})\) is deduced from its matrix, for each of the beam spots from the probe array. For relative positioning of the beam spot array, all the \((a_{sb}, b_{sb})\) points are used to construct effective relative coordinates, which provide a reference for operation in near-field applications.

In this study, to realize conditions similar to a practical circumstance, ideal locations are defined in an \(N \times N\) square matrix, and random noise is applied. The pixel number is enough to describe the diffracted optical image of the isolated spot pattern, but the obtained position of a spot pattern has position errors by the effective pixel size \((p)\) based on the magnification of the objective lens. Each spot pattern location identified based on the optical microscope image has errors of pixel-size order. However, through the recognition of the center point on the diffracted spot pattern distribution, position error is reduced to value less than pixel size. Nevertheless, for analysis, we defined the error range as \(-p < \text{position} < p\) with maximum discrepancy of \(2p\). Random noise is generated on the basis of a normal distribution with a maximum deviation of \(p\) \(p = 60\) nm with

\[
X_n = d \theta y_{X_n} + 2a.
\]

\[(2.4)\]
a 0.95 NA objective lens). It is expected that the considered error range could be enough to be evaluated with a near-field optical system. The left-right and top-down directions along the picture are defined as the x- and y-axes, respectively. After implementing the above methodology in sequence, linear regression analysis is used to infer the ERP of each matrix, which is regarded as the representative value of each probe. Figure 3 shows the results of this process for a matrix of \( N = 11 \). Both \( a \) and \( b \) can be simply obtained, as shown in the graph of Fig. 3.

3. NUMERICAL ANALYSIS

This method can accurately identify the relative position values of the beam spots with higher probability than the simple method of directly reading the spot position, which incorporates the error range determined by the pixel size. To confirm the feasibility of the proposed methodology, we evaluate its accuracy and uncertainty using numerical analysis.

A. Accuracy of Methodology with Random Noise

Combined with random noise, we estimate the accuracy by verifying the standard deviation \( \sigma \) of the calculated \( a \) relative to the ideal location, as shown in Fig. 4(a). We numerically analyze \( \sigma \) as a function of the number \( N \) along lateral direction in a spot pattern array having a square matrix arrangement.

Because the same level of random noise is distributed in both the x- and y-directions, the variation of \( a \) on the x axis only is described. The position matrix, which has identical ideal points, is affected by the random noise, and the process described in the previous section is employed to determine the value of \( a \). By repeating the calculation process, the deduced \( a \) values are spread over a certain distribution. A reliable dispersion of \( a \) values is observed for a sufficient number of iterations, i.e., \( 10^4 \). As the variation between the average \( a \) value and the initial ideal value is less than 1 nm, the mean value is not a meaningful parameter as an evaluation standard.

We extend the number of spot patterns, i.e., the size of the square matrix with \( N \) rows and \( N \) columns, in a corresponding distribution, and determine the standard and maximum deviations of the \( a \) values with respect to the ideal location. The results obtained by varying the \( N \) values from 3 to 29 are depicted in Fig. 4(a). It is apparent that increasing \( N \) reduces \( \sigma \), and this decrease appears to be inversely proportional to the increasing number of spot patterns \( N^2 \). The appropriate value of \( N \) for the desired accuracy and its range can, therefore, be identified. Only one spot pattern for each probe can produce the standard deviations and maximum deviations of approximately 17 and 60 nm, respectively, by recognition of a point location.

B. Uncertainty of Methodology with Respect to \( N \)

It is impossible to obtain the definite ideal position of the fabricated probe array for practical demonstration. Hence, the relative position trend must be determined between the beam spots based on the reference coordinates. The deviation calculated above incorporates the errors generated by the methodology and by the use of the optical microscopy image for location identification. However, the approach for estimation of accuracy is not appropriate to evaluate the experimental results, which cannot be analyzed by definite comparison value despite the merit that shows the capability of the estimating method on the basis of the ideal case in Fig. 4. Therefore, a relative reference value needs to be defined and evaluated for comparison with the experimental outcomes.

We construct four matrices with random noise in a normal distribution with \( 2 \times 2 \) groups and deduce both \( a \) and \( b \) for the x and y axes, respectively, for relative comparison in two dimensions. A simple schematic to address the relative parameter \( P_m \) is shown in the inset of Fig. 5(a). The correlation between the representative points of the probes is presented as vector \( P_m \) with respect to Probe 4. The magnitude of \( P_m \), i.e., \( |P_m| \), which is the relative length, is calculated. The value of \( |P_m| \) includes errors due to variation from the designed pitch parameter and practical factors related to the tolerance of the probe array fabrication. Therefore, evaluation of the relative correlation confirms the fabrication errors \( \Delta F \) with nanometer accuracy in the regular state, and a realistic coordinate is established across the area covered by each probe. In numerical analysis, the tolerance due to the fabrication is assumed to be zero, and the definite accuracy of this methodology is verified. In this case, the uncertainty of \( |P_m| \) is considered in order to evaluate the precision, rather than definite comparison to the ideal value. In Fig. 5(a), \( \sigma \) and \( 2\sigma \) for \( |P_m| \) are depicted as functions of \( N \).

When \( N \) is more than 11, \( \sigma \) indicates an uncertainty of less than 10 nm with 95% probability. For two cases of \( N = 11 \) and 21, the deviation distributions (for \( a \) relative to the ideal location) are plotted in Fig. 5(b). An uncertainty of less than 5 nm can be achieved with \( N > 21 \).
4. EXPERIMENTAL RESULTS

The 2 × 2 probe array is employed in the experiment to confirm the feasibility of the methodology in practical application. The probes are separated by a 150-μm pitch, and a bowtie-shaped nanoaperture with an outline of approximately 150 nm and a gap of 20 nm is perforated in the end of each pyramidal probe. The fabricated probe array and nanoapertures are measured by scanning electron microscopy (SEM), as shown in Fig. 6. The optical source, which is a laser with 405-nm wavelength, is incident on each probe via a microlens array and project optics. PR (Dongsin Semichem, DPRi-7201) is deposited with 100-nm thickness on a Si wafer with dimensions of 1 cm × 1 cm. Using a condition to generate a pattern with a diameter of 300–500 nm, which is the appropriate size to provide sufficient pixels, a 12 × 12 array of spot patterns is recorded in PR with 2-μm displacement. If a spot pattern is too small, the number of recognized pixels is insufficient, and it becomes difficult to determine the location of the center point in a spot pattern. The developed pattern is measured by a conventional optical microscope with a 100 × objective lens. The sample is aligned and captured into image data with 1024 pixels × 1280 pixels of 60 nm in size, as shown in Fig. 7(a). The aforementioned analytical process is performed using the MATLAB tools code, as shown in Fig. 7(b). Figure 7(c) shows the linearly fitted results for $X_n$ and $Y_n$ as functions of $\gamma$ for Probe 4. The data scattering has a tendency similar to the noise-added data used in the numerical analysis.

The ERPs of the 2 × 2 probe array are induced as $(a_k, b_k)$ coordinates and the $|P_1|$, $|P_2|$, and $|P_3|$ correlation parameters are calculated. Because a 12 × 12 matrix is obtained for each probe, the $N$ that can be analyzed is an odd number less than 12. At least four data points can be calculated for each $|P_m|$, with the value of $N$ in the spot pattern being varied; therefore, matrices with $N$ values of 3 – 11 can be estimated. The maximum and minimum $\sigma$ values for $|P_m|$ are compared with the numerical analysis results, as shown in Fig. 8.

The deviations obtained in the experimental demonstration are lower than those with the random noise. The experimental error is complexly affected by various background unknowns due to the scanning operation and interaction between the probe, substrate, and stage. The effect by alignment of probe and substrate is geometrically estimated to be less than 1 nm, and the lateral movement error is also assumed to be less than 1 nm under contact conditions as a result of the symmetric probe design. It is thought that no location error is induced by the scanning process, because we operate the probe with...
a dot-printing mechanism for patterning. The error induced by the movement of piezo stage is not considered. The numerical analysis assumes that all effects mentioned above are fully incorporated within the random noise. The distribution of the experimental $X_n$ and $Y_n$ values with variation of $\gamma$ is confirmed in Fig. 9(c) and can be compared with Fig. 3. Similar distributions can be observed for both figures, but in many cases, the experimental results are less scattered. For the numerical analysis, a large number of possible samples were considered and calculated with a probability distribution, but in the experimental demonstration, a limited amount of data was analyzed for understanding the relation of beam spots with lower uncertainty less than numerical $\sigma$ in the section of high probability.

The relative distance between the beam spot locations shows the variation in response to realistic movement of the stage. Thus, there is a discrepancy between the positions in the real probe array compared to the design values, due to both $\Delta F$ and the methodological errors. Therefore, the finally obtained effective relative locations include both the designed geometrical values and the $\Delta F$. They construct a modified reference coordinate system so that patterns can be generated across a different probe area. The sequential process for defining the positions and the continuous patterning process are performed in adjacent areas by more than two probes.

To demonstrate the feasibility in application of near-field lithography, we performed both relative positioning and patterning in a serial process. Using a fabricated probe array, spot array patterns were generated for the position matrices with $N = 9$ yielding ERPs. Depending on the proposed method, obtained ERPs construct the relative coordinate system for probes to each other. The estimated $\Delta F$ for used probe array ranges from 100 to 300 nm to be considered in coordinates. Based on determined position values, we can control the beam spot location of the probe array for design of the lithographic target pattern.

**Fig. 7.** (a) Captured optical microscope image of $12 \times 12$ spot-array patterns; (b) data processing with MATLAB program for inducing ERP; (c) linear regression of $(\gamma X_n, X_n)$ and $(\gamma Y_n, Y_n)$ with results of Probe 4.

**Fig. 8.** Experimental result uncertainty compared to that for numerical analysis results. The results are well matched to the random noise case, as indicated by the estimated $\sigma$.

**Fig. 9.** Application of methodology to parallel lithography. Optical microscope images of (a) $3 \times 3$ spot array patterns formed with $2 \times 2$ probe array, based on coordinates constructed using calculated positions; (b) arbitrary pattern of cow-head structure created by $2 \times 1$ probe array; (c) linear regression process with $(\gamma X_n, X_n)$ and $(\gamma Y_n, Y_n)$ experimental results by matrices of $N = 9$.
As shown in Fig. 9(a), each beam spot from each probe makes the $3 \times 3$ spot-array pattern and four groups of patterns by $2 \times 2$ probe array are overlapped with each other group along the border line. Also, with two inverted images, cow-head arbitrary structures are patterned in the boundary area with a pattern width of $\sim 200$ nm by each of two probes [Fig. 9(b)]. Depending on the locations obtained by ERP's, each near-field beam spot from each bowtie aperture can be exposed appropriately at the point to be desired. Based on the above analysis results, we estimate that a matrix with $N = 9$ can yield relative coordinates with an uncertainty of less than approximately 5.5 nm with a probability of 68.2%, and an uncertainty of less than 11 nm with a probability of 95.4%. In this case, the precision values could be less than 5.5% of the pattern size.

Depending on the desired level of stitching error, the appropriate $N$ can be selected for a certain level of uncertainty. A simple spot pattern gives rapid feedback for obtaining the location information employed to produce the pattern design. It is expected that, at $N$ values greater than 21, an uncertainty of less than 5 nm can be maintained with a probability of 95.4%.

5. CONCLUSIONS

An extended beam source in the form of a two-dimensional array has been developed for near-field technology. Therefore, it is necessary to define and assign the position of each beam with high precision. We have identified the relative coordinates of the beam spots using a methodology proposed in this study. The ERP for each probe is determined based on the position matrix constructed by the spot array patterns with a lithographic technique and obtained by linear regression using a series of derived equations. The data are based on an image captured by a conventional optical microscope; thus, this method has the advantages of time efficiency, a simple process, and fast feedback. It is not easy to verify a near-field beam array with micrometer pitch using high-resolution measurement technology, such as an atomic force microscope or a SEM, because of their working areas. Therefore, in order to validate our proposed relative-position analysis method, we calculated the accuracy and uncertainty of both numerical and experimental results obtained using the devised method. Both sets of results are in good agreement with respect to the uncertainty, which implies that our method works well. Furthermore, we applied the proposed method to a parallel lithography process for multiarea patterns. The approach was successfully demonstrated for patterning using a near-field beam array as determined by the relative coordinates. We expect that this method can provide an uncertainty of less than 5 nm with an optimal spot pattern position matrix, thereby facilitating effective use of near-field beam sources for extensive application via relative positioning analysis.

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