Deep Groove Measurement using Broadband Opti cal Frequency Comb Scattering Spectroscopy

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We have been developing a method for measuring fine surface topography over a wide area with high accuracy using the laser inverse scattering method. The laser inverse scattering method has been reported as a method for measuring surface topography with sub-micrometer dynamic range by illuminating a monochromatic plane wave perpendicular to the target surface and retrieving the phase distribution of the reflected light. In this study, we aim to extend the dynamic range of the laser inverse scattering method to the micrometer order by using an optical frequency comb. However, multiple waveguide modes are generated in the groove whose depth is deeper than the incident wavelength, and the phase distribution does not reflect the surface topography. Therefore, we have developed a method to obtain a phase distribution that more accurately reflects the surface topography by correcting the electric field at the groove aperture using the analytical solution of the generated waveguide modes. In this paper, the validity of the proposed method is confirmed by numerically analyzing and correcting the phase distribution of the scattered electric field on a rectangular groove surface with a monochromatic plane wave incident on it.

NOMENCLATURE

 λ = wavelength h = surface topography n = the number of phase shift θ = phase distribution of a scattering light k_0 = incident wave number $k_{x,z}$ = wavenumber in x,z direction m = order of waveguide mode μ_r = specific permeability

1. Introduction

In recent years, the demand for ultraprecision optical elements such as aspherical lenses and diffraction gratings, which are key components of digital cameras, optical disks, and exposure devices used in semiconductor manufacturing, and their molds has increased. In response, ultra-precision machining technologies have been rapidly developed, and machining is carried out with shape accuracy in the order of 10 nm. To realize such high-precision machining, in-process measurement is required to measure the surface profile during machining and to feed back the measurement results to the machining process in real time. Therefore, the 3D surface profiling technology must be fast, accurate, and robust against target vibration.

Typical 3D surface profiling techniques include scanning probe microscopy, stylus roughness measurement, scanning white light interferometry, and confocal microscopy. However, these measurement methods are not suitable for in-process measurement because of their low robustness due to sensitivity to the vibration of the measurement target. On the other hand, laser inverse scattering method has been reported as a 3D surface topography measurement technique that is robust against vibration [1].

When a monochromatic plane wave is illuminated on the target surface, the reflected wavefront coincides with the surface profile of the target. The laser inverse scattering method measures the surface topography of the entire illuminated area by obtaining the intensity distribution of the surface image and the Fraunhofer diffraction pattern, and retrieving the phase distribution of the scattering light generated on the target surface from these intensity distributions. The intensity distribution of the diffraction pattern depends on the spatial frequency of the target and is not affected by target vibration, allowing robust surface measurement against vibration.

However, if the acquired phase distribution exceeds $[-\pi, \pi]$, it is wrapped within $[-\pi, \pi]$ and has discontinuous shifts. Since the number of phase shifts cannot be calculated by phase retrieval, the dynamic range of the laser inverse scattering method using a single wavelength laser is limited to the sub-micrometer order. In this study, we aim to extend the dynamic range to the order of micrometers by using an optical frequency comb as a light source and estimating the surface topography from changes in the phase distribution for multiple wavelengths. However, in a groove whose depth is deeper than the incident wavelength, multiple waveguide modes are generated and the retrieved phase distribution is inconsistent with the surface topography, resulting in a reduction in the accuracy of the surface topography measurement. In particular, it is important to improve the measurement accuracy of the rectangular groove, which is the basic shape of various optical elements such as diffraction gratings and light guide plates.

On the other hand, a method to obtain the analytical solution of the scattered electric field at the aperture of a rectangular groove as the sum of multiple waveguide modes has been reported [2]. Therefore, we have developed a method to obtain a phase distribution that accurately reflects the surface topography by using the analytical solution of the scattered electric field to remove the phase modulation caused by higher-order waveguide modes from the retrieved phase distribution.

In this paper, we confirm the validity of the phase correction method by correcting the retrieved phase distribution obtained from the numerical analysis of the scattered electric field on the rectangular groove surface.

2. Principle of deep groove measurement using optical frequency comb and correction of phase modulation

Figure 1 shows a surface topography measurement based on the laser inverse scattering method using an optical frequency comb as a light source. When a plane wave of wavelength λ_i is vertically incident on a sample with surface topography h(x, y), scattering light with phase distribution $\theta_i(x, y)$ is generated. In this case, the relation between θ_i and λ_i is

$$\theta_i(x, y) = 2\pi \left\{ \frac{2h(x, y)}{\lambda_i} - n_i(x, y) \right\},\tag{1}$$

where $n_i(x, y)$ is the number of phase shifts. The scattering light is formed as a Fraunhofer diffraction pattern at the back focal plane of the objective lens and as a surface image of the sample at the focal plane of the imaging lens. The surface image and diffraction pattern are spectrally analyzed to obtain the intensity distribution of the surface image and diffraction pattern for each wavelength component. The Gerchberg-Saxton method (hereafter referred to as GS method) [3] is then used to retrieve $\theta_i(x, y)$ for each λ_i from these intensity distributions. The algorithm iterates the Fourier transform between the spatial and frequency domains, using the intensity data measured in each domain as constraints. To avoid convergence to a local solution and to reduce solution ambiguity, a phase distribution constructed based on a priori knowledge is used as the initial phase. The phase distribution obtained by the GS method is wrapped around the principal value $[-\pi, \pi]$, and the number of phase shifts is unknown. Therefore, the laser inverse scattering method using a single-wavelength laser can only measure shapes with subwavelength height. However, since the retrieved phase distribution is inversely proportional to the wavelength, h(x, y) can be estimated from the phase distribution at multiple wavelengths, thus extending the dynamic range of the laser inverse scattering method in the height direction.



Fig. 1 Surface topography measurement using optical frequency comb.

On the other hand, multiple waveguide modes are generated in the groove deeper than the incident wavelength. When a monochromatic plane wave is vertically incident on a rectangular groove as shown in Fig. 2, the transverse modes are confined by the groove wall while the electromagnetic field scattered at the groove edge propagates. In this case, the boundary condition $E_y(\pm D/2) = 0$ results in the x-axis wavenumber $k_x = m\pi/D$ ($m = \pm 1, \pm 3, \pm 5, ...$), where m is the mode order. Therefore, the relationship between the wavenumber $k_{x,z}$ in the x, z direction can be expressed as

$$k_0^2 = k_x^2 + k_z^2 = \left(\frac{m\pi}{D}\right)^2 + k_z^2.$$
 (2)

When multiple waveguide modes are generated, the electric field at the sample surface is the interference of each mode. The phase of each mode wave as it travels back and forth in the groove is different for each mode, so when multiple waveguide modes are generated, the phase distribution of the electric field on the sample surface is not consistent with the surface topography. Therefore, it is necessary to correct the phase modulation caused by the waveguide modes generated in the groove. When a monochromatic plane wave is vertically incident on a rectangular groove as shown in Fig. 2, the electric field E_v at the sample surface z = 0 at $|x| \le D/2$ is

$$E_{y}(x,0) = E_{0} \sum_{m=1}^{M} \frac{4k_{0}\mu_{r}}{m\pi k_{z}} \sin\left\{\frac{m\pi}{D}\left(x+\frac{D}{2}\right)\right\} e^{-2ik_{z}h}, \quad (3)$$

which is obtained in [2]. Note that M is the highest order of the mode generated in the groove, and μ_r is the specific permeability of the material filling the groove and the top of the groove. Since the lateral resolution of the laser inverse scattering method depends on the diffraction limit of the optical system, the surface topography with a lateral shape on the order of micrometers is targeted for measurement in this study. When the groove width is sufficiently larger than the incident wavelength, the wave number of the first-order waveguide mode $k_z \approx k_0$, and the phase distribution of the electric field of the first-order waveguide mode is in good agreement with the surface topography. Therefore, by subtracting the waveguide modes of $m = 3 \sim M$ from the electric field obtained from the surface image and the retrieved phase distribution, a phase distribution reflecting the surface topography can be obtained. Note that the dimensions of the design shape used for phase retrieval are used as the groove parameters to be substituted into Eq. (3). As described above, by correcting the phase at each wavelength of the optical frequency comb, the surface topography can be estimated more accurately from multiple corrected phase distributions.



Fig. 2 Geometry of a rectangular groove.

3. Correction simulation of the phase distribution of scattering light on a rectangular groove surface.

To confirm the validity of the proposed method, the phase distribution obtained by electromagnetic field simulation was corrected by the proposed method, and the corrected phase distribution was compared with the uncorrected phase distribution.

In the electromagnetic field simulations, the FDTD method was used to calculate the electric field amplitude and phase distribution on the surface of a rectangular groove when a plane wave with 450 nm in wavelength was incident on the groove. To confirm the validity of the proposed method for grooves with different aspect ratios, the groove depth and width were set to 1 µm and 1~10 µm, respectively. The far-field electric field was obtained by Fourier transforming the complex amplitude expressed by the electric field amplitude and phase distribution. This far-field electric field is both the electric field on the back focal plane of the objective lens and the spatial frequency spectrum of the electric field on the surface of the rectangular groove. In the actual measurement, scattering light that does not pass through the objective lens does not contribute to the formation of the surface image or diffraction image because the diameter of the objective lens is finite. Therefore, the spatial frequency spectrum larger than the cutoff frequency $f_c = N.A./\lambda$ is set to 0. The inverse Fourier transform of the filtered spatial frequency spectrum was used as the electric field amplitude of the rectangular groove surface. N.A. is the numerical aperture of the objective. The phase retrieval was performed by the GS method using the electric field amplitude of the rectangular groove surface and the filtered spatial frequency spectrum. In this experiment, the N.A. of the objective lens was set to 0.55. When calculating the electric field at the groove surface using equation (3), $\mu_r = 1$ in the groove and at the top of the groove, and $E_{\nu}(x, 0) =$ 1 + 0i for D/2 < |x|. The analytical solution was also filtered in the spatial frequency domain to obtain an analytical solution for the electric field at the groove surface, taking into account the finite lens aperture.

Figure 3 shows the electric field amplitudes at the groove surface obtained by the FDTD method and calculated from eq. (3) for groove widths of 3, 6, and 9 μ m. In Fig. 3, the electric field obtained by the



Fig. 3 Electric field amplitudes at the groove surface obtained b y the FDTD method and analytical solution for groove widths (a) 3, (b) 6 and (c) 9 μ m.

the scattering phenomenon at the edge. The electric field in the groove is wavy with multiple peaks, and the number of peaks in the electric field increases as the groove width increases. This is due to the increase in the number of waveguide modes generated in the groove as the groove width increases. The electric field in the groove obtained by the FDTD method and the analytical solution obtained from eq. (3) are in good agreement. From the above, it has been confirmed that eq. (3) can be used to calculate the electric field at the groove aperture where multiple waveguide modes are generated.

The retrieved phase distributions at groove widths of 3 and 5 μ m, the corrected phase distribution using the sum of third-order and higher waveguide modes, and the theoretical values are shown in Fig. 4. Figure 4(a) shows that the retrieved phase distribution for a groove width of 3 μ m rises near the edge, and the phase beyond π is wrapped. Because the surface image and diffraction pattern used for phase retrieval are filtered in spatially frequency domain and have no information about the vertical convexity of the phase distribution, a phase distribution with a continuous and upward convex profile at the edge is retrieved. The corrected phase distribution has a narrower area corresponding to the bottom surface than the uncorrected phase distribution, which reflects the surface topography less accurately. This

FDTD method decreases to about 0.2 V/m near the edge, confirming

is due to the subtraction of the sum of the third-order or higher waveguide modes calculated under the assumption of a bottom-convex phase distribution from the electric field with a top-convex phase distribution.



Fig. 4 Uncorrected, corrected phase distribution and theoretical v alues for groove widths of (a) 3 and (b) 5 μ m.

The retrieved phase distribution with a groove width of 5 μ m showed a convex distribution downward that gradually narrowed, and a wavy distribution with three peaks was observed in the area corresponding to the groove bottom. The corrected phase distribution decreased more steeply near the edge than the uncorrected phase distribution, reflecting the edge of the groove bottom.

To confirm that the proposed method produced a phase distribution that more accurately reflected the shape near the edge, the distance from the position of the maximum value on the top surface of the groove to the position of the minimum value on the bottom surface of the groove in the region near the edge of the phase distribution was calculated as the edge region. To confirm the agreement of the corrected phase distribution with the surface topography, the mean square error of the entire phase distribution and the theoretical value were calculated. The edge area is shown in Fig. 5 and the mean square error is shown in Fig. 6. Figure 5 shows that the edge area decreased except for groove widths of 2, 3, and 7 μ m, with a maximum decrease of 1.33 µm at a groove width of 10 µm. The increase in the edge area at groove widths of 2, 3, and 7 μ m is due to the fact that the retrieved phase distribution was convex upward as in Fig. 4 (a), and thus the phase distribution was not properly corrected. Figure 6 shows that the mean square error between the corrected phase distribution and the theoretical value is less than or equal to that between the uncorrected phase distribution and the theoretical value, except for groove widths of 3 and 7 µm. Therefore, the proposed method does not degrade the consistency between the phase distribution and the surface topography. Thus, it was confirmed that the proposed phase correction method can obtain a phase distribution that more accurately reflects the surface topography, especially near the edges.



Fig. 5 Edge areas of the uncorrected and corrected phase distributions.



Fig. 6 Mean squared error of uncorrected and corrected phase d istributions relative to theoretical value.

4. Conclusions.

In this paper, we propose a method for phase correction in surface topography measurements by laser inverse scattering using an optical frequency comb. In the proposed method, the phase is corrected by subtracting the sum of third-order or higher waveguide modes from the electric field at the groove aperture. The phase distribution of the scattered electric field when a monochromatic plane wave is injected into the rectangular groove calculated by the FDTD method is corrected, and the corrected phase distribution is compared with the uncorrected phase distribution. The corrected phase distribution more accurately reflects the surface topography, confirming the validity of the proposed method.

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