Near field modeling of the Moiré interferometer for nanoscale strain measurement

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Abstract

In this study, we propose a new method to validate the basic assumptions used in Moiré Interferometry (MI) measurement using exact electromagnetic (EM) theory, and simulate the EM fields in a few microns region above the surface of the diffraction grating. Proving that spatial frequency of EM field matches the spatial frequency of strain field is critical to ensure accuracy of MI measurement at nanoscale resolution. The EM simulations for a deformed diffraction grating structure were performed by introducing a single defect that acts as a variation on the periodic diffraction grating. The spatial frequency of simulated EM field was quantified using Continuous Wavelet Transform (CWT) algorithm. The results were compared with the strain field to show the correlations between the two. The study shows that there is a strong correlation (correlation factor $R = 0.869$) of spatial frequency response between EM field and strain field at the nanoscale. The study shows that using the traditional MI assumptions for nanoscale strain measurement introduces an error in the order of 2.7%. We demonstrate that MI measurement can be used for nanoscale strain measurement within acceptable measurement errors using the proposed method. The proposed method can help to evaluate the MI instrument design to enhance the measurement performance.

1. Introduction

The continuous miniaturization of the electronics requires advancement of metrology to enable research and development of electronic and photonic devices with nanoscale features [23]. The understanding of the mechanical behavior of nanoscale devices is critical to their development and reliability testing [24,42,48]. Moiré Interferometry is a full field strain map measurement technique and has been successfully applied to study mechanical behaviors of different structures with different material composition [5,7,39,57,58]. Recently it has been used extensively to study the thermal mechanical behavior of semiconductor devices and their packaging [19,21]. The concept of nanoscale strain has been proposed from several studies when the strain fields are presented on deformed structures defined by their nanoscale features (feature size ranging from 20 nm to 400 nm) [9,32]. When using Moiré Interferometry for nanoscale measurements, using the wrapped front theory [10] lacks the ability to interpret the behavior at nano-scale because of strong diffraction effect caused by nanoscale features. In order to measure the strain field with nanoscale resolution, it is important to understand the degree of the correlation between the strain field spatial frequency and electromagnetic field spatial frequency because any discrepancy will introduce error into the measurement. If the correlation relationship between the spatial frequencies of the two fields is known, the uncertainty and the error in the strain measurement can be better quantified. Furthermore, understanding the near-field electromagnetic field interaction with Moiré diffraction grating is essential to design high sensitivity nano resolution Moiré interferometer based on different principles, for example, near-field optical microscopy [13], far-field super-lens based microscopy [33] and far-field phase shifting interferometry [5,6].

In the literature, state-of-the-art nanoscale strain measurement techniques can be categorized by their microscopy methodologies and their deformation detection techniques. The microscopy for nanoscale strain measurement is mostly either Scanning Probe Microscopy (SPM) or Scanning Electron Microscopy (SEM). The most common deformation detection techniques include: (1) Moiré Interferometry (MI) and (2) Digital Image Correlation (DIC). also reported using Atomic Force Microscopy (AFM) combining with DIC to achieve nanoscale strain/displacement measurement [45]. Sutton et al. reported that 1 nm displacement measurement was achieved using scanning electron microscope (SEM) combining with DIC technique [46,47]. Xie et al. proposed a phase shifting SEM Moiré technique to measure the nanoscale deformation using 6000 lines/mm diffraction...
grating fabricated by electron beam lithography [56]. Xie et al. also proposed an AFM Moiré method [55]. Holographic interferometry using Transmission Electronic Microscope (TEM) has been reported for nanoscale strain measurement with the application on strained silicon substrate [22]. However, these techniques can only measure the strain field in an area with edge length of 1 µm. Moreover they etch the sample with focused ion beam or electron beam lithography which does introduce damage to the surface of the sample. In order to apply Moiré Interferometry (MI) on nano-scale strain measurement, it is important to have a near field model of MI, which can be used to study surface structure interactions with the scattering of waves in the near field region of a metallic grating. In this study, we focus on the electromagnetic waves instead of particle waves (e.g., electron beams). The near field modeling helps to validate the basic assumption used in scalar wave diffraction theory (i.e., Kirchhoff’s formulation and Rayleigh–Sommerfeld formulation of diffraction) [17], which can be used to model and simulate behaviors of interferometers [20]. In addition, this study also lays the groundwork for integrating super lens and scanning probe microscopy with Moiré Interferometry for nano-scale full field strain measurement [15,33].

The purpose of this study is to establish a correlation between the spatial frequency information on the surface relief grating structure and the one encoded in the near field electromagnetic waves. It is documented that the spatial frequency (or instantaneous frequency) is the essential information for strain measurements in MI [26,27]. The spatial frequency information is extracted using Continuous Wavelet Transform (CWT), which is widely used in the interferogram processing [30,31]. Geometrical variations or defects are introduced into the periodic surface relief grating structure; and then electromagnetic field within 5 µm hemisphere is calculated using Finite Element Method (FEM). Both Finite Difference Time Domain (FDTD) and FEM are extensively used for numerical calculation of electromagnetic fields. FEM is chosen in this study because, the flexible meshing scheme in FEM gives better efficient on solving the problems with large geometrical complexity [25]. The study shows that the defect with sub-wavelength size is able to introduce correlation of the spatial frequencies.

2. Classical theory of Moiré Interferometry and challenges at nanoscale

The basic configuration of Moiré Interferometer (MI) is shown in Fig. 1. In order to measure two orthogonal displacement components simultaneously, most of MI systems are set up with four coherent He–Ne laser (λ = 632 nm) beams [39]. However, since four beams follow a rotational symmetry, we limit our discussion here in a two-beam arrangement. As shown in Fig. 1, two coherent laser beam denoted by their directive vectors, \( k_1 \) and \( k_2 \), are positioned at the specific angles so that +1 diffraction order \( k'_1 \) of the \( k_1 \) beam and −1 diffraction order \( k'_2 \) of the \( k_2 \) beam are output almost perpendicular to the surface grating on the specimen. The classical theory of Moiré interferometer (MI) based on warped wavefront model was first proposed by Dai et al. [10].

The general idea of warped wavefront model is that the deformation information can be obtained from the phase of diffracted waves \( k'_1 \) and \( k'_2 \). McKelvie extended the theory and applied it on the analysis of sensitivity and resolution limitation of MI [36]. Here Dai and McKelvie’s approach is briefly reviewed. The 1D diffraction equation can be written as [34]

\[
\begin{align*}
    k'_x &= k_{ox} + 2\pi f_x n_x \\
    k'_z &= k_{oz}
\end{align*}
\]

(1)

where \( k_{ox}, k_{oz} \) are the components of incident wave vector \( \vec{k}_1 \), \( \vec{k}_2 \), \( k'_{ox}, k'_{oz} \) are the components of diffracted wave vector \( \vec{k}'_1 \) with the

![Fig. 1. Schematic of the working principle of Moiré Interferometry with a two-beam arrangement, where \( k_1 \) and \( k_2 \) are incident laser beams. The diffraction orders for both beams are shown. The +1 diffraction order of \( k_1 \) incident beam is designated as \( k'_1 \), and the −1 diffraction order of \( k_2 \) incident beam is designated as \( k'_2 \).

where \( f_x \) is the original spacing frequency of the grooves on the surface grating along the x-direction. For the most commonly used Moiré grating the spacing frequency of the groves is 1200 lines/mm; and it is the equivalent to \( f_x \approx 833.3 \text{ nm} \).

Assuming that the incident beams are ideally collimated, the incident beams then can be modeled using plane wave equations without considering non-linear optical interaction and frequency dispersion, which is shown as in Eq. (2).

\[
E_i = A\exp(i k_1 \cdot \vec{x})
\]

(2)

where \( E_i \) is the electrical field of the wave, \( A \) is the absolute amplitude of the plane wave, \( k_1 \) is the directional vector of the incident waves with \( i = 1, 2 \), and \( \vec{x} \) is the spatial coordinate vector with components \( (x,y,z) \).

It is assumed that there is phase change in the diffracted beam. As a result, electrical field equation becomes,

\[
E'_i = A\exp[i(k'_1 \cdot \vec{x} + m_1 f'_x(x,y) + m_2 f'_y(x,y) + m_3 f'_z(x,y) + m_4 f'_z(x,y))]
\]

(3)

Where \( f'_x(x,y) \) is the spacing frequency of the deformed grating along the x-direction.

This assumption allows modeling MI without solving Maxwell’s equation and the integrals in Rayleigh–Sommerfeld or Kirchhoff’s solutions for the scalar wave equation. However, the approximation introduced by the latter assumption becomes uncertain when the dimensions of the measured features approach nanoscale. The reason is that the latter assumption leads to generic treatment of diffraction using only the generalized diffraction equation. In addition, the assumption cannot accommodate aberration of lens in the imaging system. The intensity of the interference pattern \( I \) can then be calculated...
using Eq. (4)
\[ I = (E_1 + E_2)(E_1^* + E_2^*) \]  
(4)
where \((\cdot)^*\) denotes the complex conjugate of a function.

By considering the initial incident angle, introducing Eq. (3) into Eq. (4); and the intensity of the interference can be rewritten in terms of the spatial frequency function \(f_s\) of the deformed grating, as shown in Eq. (5):
\[ I = 2A^2(1 + \cos(4\pi(f_s - f_{s0})\lambda)) \]  
(5)

One advantage of wrapping wavefront model is its simplicity. The conclusion (refer to Eq. (5)) can be readily used for deformation calculation in the fringe counting method [18] and can also be used to interpret basic phenomena in MI (i.e., null field). However, the warped wavefront model itself suffers from the over simplification of the treatment of the near field diffraction and the wave propagation over free-air. To overcome this problem, the near field modeling based on Maxwell equations offers better solutions and will be explored in this study.

3. Electromagnetic theory and finite element formulation

In this section, we will briefly review the electromagnetic theory and finite element formulation. The purpose is to iterate all the basic assumptions made during the formulation process, which imposes certain degrees of restrictions on the material property, and geometrical configurations. Although the approximation made during the computational simulation process reduces the computational complexity of the problem, it also restricts the applicability of the model itself. However, the principal objective is to build a flexible near field computational model for Moiré Interferometry (MI) while maintaining the accuracy at the nanoscale.

In computational electrodynamics, it is costly and inefficient to solve the full Maxwell’s equations especially when the high frequency optical wavelength is involved. In MI, the iodine-stabilized helium-neon (He–Ne) laser operating at 633 nm is the most commonly used single mode laser source. He–Ne laser offers very narrow bandwidth at its operating wavelength [29], which can be treated as a single frequency electromagnetic radiation source when it is modeled. Therefore, instead of using full Maxwell’s equations, the time harmonic Maxwell’s equation is more applicable here, which removes the time component and considers only one single wavelength. Assuming isotropic material constitutive relation, the time harmonic Maxwell’s equations are written as shown in Eqs. (6) and (7) [25].

\[ \nabla \times \mathbf{E} = j\omega \mu \mathbf{H} \]  
(6)

\[ \nabla \times \mathbf{H} = -j\omega \varepsilon \mathbf{E} \]  
(7)
where \(\mathbf{E}\) is the time harmonic electric field vector in V/m, \(\mathbf{H}\) is the time harmonic magnetic field vector in A/m, \(j\) is the time harmonic electric current density in A/m², \(\omega\) is the angular frequency in rad/s, \(\varepsilon\) is the permittivity tensor in F/m, \(\mu\) is the permeability tensor in H/m, \(\nabla \times (\cdot)\) is the curl vector operator and \(j\) is the standard imaginary unit.

By combining Eqs. (6) and (7), we get the inhomogeneous vector wave equation as shown in Eq. (8). It can further be reduced when the problem domain involves only homogeneous medium, where both the permittivity and permeability are constant. Applying the Gauss’ law and the vector calculus identity, we derive the Helmholtz equation as shown in Eq. (8) and finally Eq. (9).

\[ \nabla \times (\mu^{-1} \nabla \times \mathbf{E}) - \omega^2 \varepsilon \mathbf{E} = -j\omega \mathbf{j} \]  
(8)

\[ \nabla^2 \mathbf{E} + k^2 \mathbf{E} = j\omega \mu \mathbf{j} \]  
(9)
where \(\varepsilon\) is the permittivity constant in F/m, \(\mu\) is the permeability constant in H/m, \(k = \omega(\varepsilon \mu)^{1/2}\) is the magnitude of the wave vector.

For solving a electromagnetic boundary value problem, especially for the diffraction scattering problem of the surface relief grating structure, there are several popular methods including finite difference time domain (FDTD) method [14,54], rigorous coupled wave analysis (RCWA) method [43] and also finite element method (FEM) [12]. RCWA is widely used for simulation of periodic grating structure with multiple layers of dielectrics [37]. FDTD and FEM are preferred when solving the grating structures with defects. Both of them perform discretization on the problem domain to enable the modeling of complex structure with different material composition. In comparison with FDTD, FEM can easily be implicitly formulated in the frequency domain. For our study, we are modeling the system on a single frequency. Therefore FEM is better suited for this study. In the electromagnetic scattering problem, the problem domain is infinite considering the continuum spaces where the electromagnetic wave can travel. The computational complexity follows \(O(x^3)\) with respect to the space. Moreover, the convergence of FEM solution depends on the mesh fineness, which is closely related to the wavelength over feature sizes ratio in the diffraction problem. In order to successfully apply FEM, the problem domain must be truncated according to the nature of the problem (i.e., considering the frequency response over the problem boundary); and also the meshing structure should be able to assure the monotonic convergence of the solution.

The geometry of the domain is defined as a hemisphere as shown in Fig. 2. Following the same condition described in the previous section, the problem is set in a 2 dimensional space \((x,z)\). The electrical field vector in the propagation domain \(\Omega\) satisfies the Helmholtz equation as shown in Eq. (9). The boundary of the main domain, denoted as \(\partial \Omega\), is consisting of two kinds of boundary conditions. One is the absorption boundary defined on \(\Gamma_w\) which

\[ E \mid _{\Gamma_w} = 0 \]  
(10)

\[ H \mid _{\Gamma_s} = 0 \]  
(11)
where \(\Gamma_w\) and \(\Gamma_s\) are incident and diffracted electromagnetic waves with the incident angle \(\beta\) and diffracted angle \(\beta\), respectively. \(R\) is the radius of the propagation sphere. Left and right sides of sphere are hidden in the schematic. The y-axis follows the same convention as in Fig. 1.
truncates the infinite unbounded propagation space into a finite domain. However, in order to maintain the equivalence before and after the domain truncation, the Sommerfeld radiation condition, as shown in Eq. (10), still need to be satisfied for the homogeneous media [25,59].

\[
\lim_{r \to \infty} (rV \times E - jkr \times E) = 0
\]  
(10)

where \(r = (x^2 + y^2 + z^2)^{1/2}\) and \(\hat{r}\) is the unit vector.

The truncated boundary can either be treated as absorption boundary condition or radiation boundary condition. Bayliss et al. developed a series of radiation boundary condition for elliptic partial differential equations with the unbounded boundary condition [2], which reduces the error comparing with directly imposing Sommerfeld radiation condition on the truncated boundary. For radiation boundary condition, the error increases when the truncated distance decreases. When considering the incident wave is in the transverse electric mode (TE mode), the first order radiation boundary condition is written as Eq. (11) according to mode-annihilating radiation boundary operator [25,28,38].

\[
\frac{\partial E_y}{\partial r} - \left( jk \frac{1}{2r} \right) E_y = 0
\]  
(11)

where \(E_y\) is the out-of-plane electrical field component and \(r\) follows the same definition as in Eq. (10).

Another way to solve unbounded boundary value problem is to construct absorption layers with matched media. The Perfectly Matched Layer (PML) proposed by Berenger et al. is one of the most utilized techniques in this category [3], which uses additional domain (called matched layer) to avoid the reflection of incident waves. The operating principle of PML is to ensure that there is no reflection on the vacuum interface when struck by an electromagnetic wave with any frequency and any incident angle. Gedney later provided a different formulation of PML using anisotropic absorbing medium [16]; and it is further generalized by Teixeira and Chew [49], which provides a Maxwellian formulation for easy implementation in FEM. The electromagnetic wave is attenuated after reaching the lossy absorbing domain governed by replacing the differentiation operator with the matched attenuated differentiation operator. Compared with the original Eq. (9), the governing equation is modified into Eq. (12) in the PML domain.

\[
\nabla_x^2 \vec{E} + k^2 \vec{E} = j\omega \mu \vec{j}
\]  
(12)

where \(\nabla_x\) is the modified operator in Cartesian coordinates and it is defined by

\[
\nabla_x = \hat{x} \frac{\partial}{\partial x} + \hat{y} \frac{\partial}{\partial y} + \hat{z} \frac{\partial}{\partial z}
\]  
(13)

where \(s_x, s_y, s_z\) are the attenuation factors.

The typical MI grating composes a glass substrate, a dielectric epoxy mold with grating profile and a metallic surface reflective coating [39], which can be gold or aluminum. In this study, the interaction between the metallic reflective coating and the dielectric epoxy layer is not modeled because of the reflection feature of the metallic coating. Therefore, the problem domain is bounded by the reflective metallic coating surface. For the metallic boundary condition \(\Gamma_m\) as shown in Fig. 2, the boundary is defined as a perfectly conducting surface, which satisfies the condition given by Eq. (14). For the propagation domain, the electrical field can be treated as a superposition of the incident electromagnetic wave \(E_i\) and the diffracted field \(E_d\) as shown in Fig. 2. In this study, \(E_i\) is a plane wave with the incident angle \(z\). For TE mode, time harmonic \(E\) satisfies the condition defined in Eq. (15).

\[
\hat{n} \times \vec{E} = 0
\]  
(14)

where \(\hat{n}\) is the inward normal unit vector on the metallic boundary surface.

\[
\hat{E}_i = \exp(jk(\sin 2\chi + \cos 2\chi))\hat{y}
\]  
(15)

To this point, the definitions of the problem domain and boundary condition are established. The approximations are made according to the common configurations in MI to ensure the accuracy of the simulation results. The infinite unbounded scattering problems are truncated so that it can be solved by FEM. The variational formulation and shape function for finite element method can be found in the reference [25]. FEM simulation provides the electrical field distribution in the near field region above the grating structure \((z < 1 \mu m)\). Beyond the near field, the electromagnetic field starts to propagate in the free space which is beyond the scope of this paper. For a far-field model of Moiré Interferometer (MI), a theory and simulation method using the mode decomposition has been proposed using the analytical formulation of the scalar diffraction theory in [5]. The near field results can be used as the initial condition in a wave propagator based on Huygens–Fresnel principle. The correlation of the spatial frequency of the diffracted electrical field and the spatial frequency of the grating profile is the fundamental principle behind MI and will be verified in the following sections.

4. Spatial frequency extraction using continuous wavelet transform

In the Moiré Interferometry (MI), the spatial frequency information, which is a characteristic of a periodic structure, is the bridge between the deformation configuration on the grating structure (presented by repeating groove patterns) and the electromagnetic field recorded in the form of interferograms (presented by orders of fringes). As explained in the previous section, under the wrapped wavefront theory, the diffracted beam can be treated as the wave function with a phase term modulated by the spatial frequency on the deformed grating as shown in Eq. (3). The intensity of the interference thus can be derived starting from Eq. (3) as shown in Eq. (5). The finite element method (FEM) used in this study provides discretized solution to the near field scattering problem; and so forth it is not in a analytical format as shown in the wrapped wavefront theory. However, the solution from FEM follows same kind of mathematical structure as a phase modulated wave function. Finally, Continuous Wavelet Transform (CWT) is introduced to quantitatively extract the spatial frequency information from both the grating structure and simulated electromagnetic field.

Watkins et al. (2007, 1997 and 1999) [51–53] show that there are several properties with CWT suitable for extracting spatial frequencies from a sinusoidal modulated signal; and the literature has reported several successful applications using it for processing optical interference fringe patterns. Heng et al. [21]; Liu [30]; Sciammarella and Kim [41] compared with the frequency domain method (e.g., Fourier transform based extraction methods), the wavelet based methods are localized both in time and frequency domain; and they give higher resolution when extracting localized phase information [30]. One dimensional (1D) CWT is used, because of the fact that grating structure is orthogonal. For 1D case, the definition of CWT is to convolute the signal with a scaling wavelet family, which can be written as:

\[
W_t(a,b) = \int_{-\infty}^{+\infty} f(t) \psi_{ab}(t) dt
\]  
(16)

where \(f(t)\) is the input signal, \(\psi_{ab}\) is the waveform function; \(a\) and \(b\) are the wavelet scaling and translational parameters, respectively, \(W_t(a,b)\) is the wavelet transformation as a function of \(a, b, f(t)\) is the complex conjugate of function \(f(t)\). The function \(\psi_{ab}\) is scaled and translated from a mother function \(\psi\), and the relationship
between them is defined as:

\[ \psi_{a,b}(x) = \frac{1}{\sqrt{a}} \psi \left( \frac{x-b}{a} \right) \]  

(17)

The complex Morlet wavelet is mostly preferred in processing interference patterns because of its sinusoidal feature weighted by the Gaussian distribution function in the frequency domain. The mother wavelet function of complex Morlet wavelet family can be written as:

\[ \psi(t) = \frac{1}{\sqrt{2\pi}} \exp(-j\omega_0 t) \exp\left(-\frac{t^2}{2}\right) \]  

(18)

where \( \omega_0 = 5.336 \) following the formulation in [50] in order to preserve the normalizaiton of the transformed result. Although the complex Morlet wavelet is not admissible in the strict sense, it can be considered admissible in a loosely satisfying sense.

Following the basic assumption made previously, the scattered electromagnetic field satisfies the format of the wrapped wave function. Taking a cross section at the distance \( z_0 \) from the top of the grating, we set the input signal as \( f(t) = \cos(\phi(t)) \). It has been shown that the point of maximum magnitude (called "ridge") of CWT \( |W_f(a,b)| \) has the following property, which is that the first derivative of the phase \( \phi \) at position \( b \) can be computed by choosing the largest response of wavelet banks [1,51]:

\[ \frac{d\phi}{da} = \frac{\omega_0}{a_{\text{max}}} \quad \text{where} \quad a_{\text{max}} \in \arg\max_{a} \left| W_f(a,b) \right| \]  

(19)

The first derivative of the phase is the spatial frequency in the field of signal processing, in which it is named as the instantaneous frequency [35]. Eq. (19) shows that the ridge of the maximum power of the CWT can retrieve the spatial frequency information.

Although CWT is an effective tool to extract the spatial frequencies, it is worthwhile to note that the estimation obtained by using CWT suffers from the errors due to the inappropriate choices of scaling factor \( a \), the finite length of the discrete input signal and the spatial discontinuity of the input signal. Nevertheless, appropriate implementation of different ridge detection schemata [4,11] can reduce the errors introduced by inappropriate choices of the scaling parameter \( a \). In the following section, the spatial frequencies extracted using CWT from both the deformed grating and the scattered electromagnetic field will be compared to examine whether a strong correlation relation could be established.

5. Simulation and numerical results

Based on the problem definition and formulations given in the previous sections, we apply the proposed method to solve the scattering problem described in Fig. 2. We carry out numerical simulations using commercial finite element simulation package COMSOL (version 4.1) with Radio Frequency Module. It is demonstrated by other researchers that COMSOL gives reliable and repeatable results for the class of properly defined boundary value problem involving the near-field high frequency electromagnetic field as long as a suitable finite element mesh is used [8,40]. Since the model is based on time-harmonic Maxwell’s equation, a single frequency \( \lambda = 632.8 \) nm is used, the reason of which is explained in the previous section. Based on our parametric study, the radius of the hemisphere 60 \( \mu \)m is needed to ensure the wave can propagate without reflection using the first order radiation boundary condition. The reason for the adoption of the radiation boundary condition instead of more common used absorption boundary condition is that the diffraction patterns beyond near-field region (called “far-field”) help to diagnose whether the finite element results are converged. If the simulation results are converging, we should see a clear diffraction pattern with correct diffraction orders. Also a separate convergence study is performed here to ensure the appropriate mesh fineness is used. The convergence plot is shown as in Fig. 3. The period is defined as \( d_o = 833.3 \) nm based upon the most commonly used 1200 lines/mm grating. The groove follows a square profile therefore the corresponding width of the groove is half of the period, which is \( w = 416.7 \) nm. The grating structure is positioned starting from the center of the hemisphere. The incident vector was set to coincide with the sphere’s axis so that indicates that the incident angle \( x \) is equal to zero.

In the simulation results of the regular grating (i.e., defects free grating), the diffraction pattern can be clearly identified by having \( m = 0 \), \pm 1 diffraction orders in Fig. 4, which again verifies that the condition of the mesh convergence is satisfied. A closer look at the electrical field around the grating region is plotted in Fig. 5.

A local defect is introduced in the grating following the same methodology used by Sun and Zheng [44], in which a single defect was introduced deliberately breaking the periodic structure of the grating. In this study, a 1 \( \mu \)m gap replaces the original 416.7 nm gap to perturb the grating structure in the way that the local spatial frequency is changed. The scattering electrical field of the defective configuration is shown in Fig. 6. Compared with the scattering pattern of the original one (see Fig. 4), the diffraction pattern and the diffraction orders remains the same. In contrast, the near field pattern shows significant changes between Figs. 5 and 7 especially near the region where the defect is introduced. In order to make more accurate comparison, the electrical field plots around the \( z = 600 \) nm cut line are produced for both the original structure and the defective one, are shown in Fig. 8. Although both Fig. 8(a) and (b) show nine peaks, the central peak in Fig. 8(b) has lower intensity but the wider spread than the corresponding one in Fig. 8(a). Since the only difference between the two configurations is the introduction of the single defect

![Fig. 3. Convergence plot of electrical field norm (V/m) versus the degree of freedom in the model (DoF). Six probing point is set along x=4 \( \mu \)m and various z positions, ranging from the near field to the edge of the scattering boundary.](image-url)
at the center of the grating profile, it is reasonable to speculate that the change in the electrical field is caused by the defect. From another aspect, the defect can be treated as the change of the localized deformation, which leads to a correlation between nanoscale deformation and the change of the scattered electromagnetic field.

In the next section, the correlation between the localized deformation and the change of the scattered field will be studied.
quantitatively by the means of the spatial frequency using Continuous Wavelet Transform (CWT).

6. Data analysis and discussion

In the previous section, it is mentioned briefly that there exists a correlation relationship between the nano-scale deformation and the detectable change in the electromagnetic field. Here a quantitative model of the correlation relationship is proposed and established, which is enabled by using spatial frequency distributions extracted by Continuous Wavelet Transform (CWT). The electrical field norm (as in Fig. 8) is input through CWT processing algorithm. The CWT power maps with the power ridge, for both the original and defective gratings, are shown in Fig. 9.

To present the complete CWT power maps, above 700 levels of the scale factor \( a \) were used to create the power ridge maps in Fig. 9. In order to remove the distortion caused by low frequency signal around the edge, the spatial frequencies were calculated using around 10,000 levels of the scale factor \( a \). The calculation results on the grating structure and the electromagnetic response before and after the deformation are presented in Fig. 10.

The spatial frequency level matches the profile of the grating structure, in which the spatial frequency can be calculated by \( f_s = \frac{2\pi}{0.833} \). The sharp change in Fig. 10(a) near the edge of the defect can be explained by the fact that, the irregularity introduced into the original periodic grating structure causes a discontinuity on the localized frequency domain. In comparison, the diffraction mechanism weakened the discontinuity in the electromagnetic field around the defect region, which is shown in Fig. 10(b).

The differences in the spatial frequency distribution near the defect region are compared in Fig. 11. We can clearly see the similarity between the patterns generated by the grating structures \( \Delta f_s(g) \) and the electromagnetic field \( \Delta f_s(E) \). Furthermore, it is significant to notice that the pulse of the electromagnetic field is wider than the one generated by the grating structures; but the spatial frequency of the electromagnetic field is relatively smaller (around 0.2 \( \mu \)m\(^{-1}\) or 2.67%). Translated into the strain measurement, it means that the strain field identified by the Moiré interferogram can be larger than the actual area on the tested specimen. Also the strain value measured may be smaller than the actual value. However, the difference should be less than 5%.
according to the simulation performed in this study. The correlation factor, which is Pearson product-moment correlation coefficient, is $R = 0.849$ between absolute values of two patterns shown in Fig. 11, which indicates that two patterns are highly correlated with each other.

### 7. Conclusions

In this paper, the spatial frequency correlation between the electromagnetic field and strain field on a surface relief grating structure were investigated and verified with a new methodology. The new methodology uses exact time-harmonic electromagnetic theory to study the near-field electromagnetic wave scattering caused by the gratings. The basic assumption of MI is that the deformation information on the grating structure is translated into the scattered electromagnetic field with an acceptable level of distortion. It is important to verify this basic assumption for MI since the interaction between the grating and the electromagnetic field, especially in the near-field region ($z \ll 1 \mu m$), has not been studied in the existing literature. The issue becomes even more significant when the strain measurement reaches the nano-scale where the size of the specimen features is near the diffraction limit. In the study, the boundary value problem set by the time-harmonic electromagnetic field has been defined and solved using finite element method. The results have been quantitatively analyzed using contiguous wavelet transform algorithm to extract the spatial frequencies information.

It is verified that the single defect introduced into a grating structure stimulates a corresponding spatial frequency change in the scattered electromagnetic field in the near field region. The patterns of the spatial frequency differences before and after the deformation are compared and showed strong correlation (correlation factor $R = 0.867$). Deviation from the existing wrapped wavefront theory is small. The spatial frequency change is smaller in the electromagnetic field is smaller than the equivalent strain on the grating by 2.67%. However, it is in an acceptable error range (i.e., $\pm 5\%$) when measuring strain at nanoscale. In Fig. 11, it is observed that EM spatial frequency value varies over a wider domain than actual grating spatial frequency. This may have been due to the discontinuities caused by the defect.

This method can serve a design tool for future nano-scale strain measurement techniques using the Moiré Interferometry. It also provides a numerical simulation method to quantifying the measurement errors and help to gain more insight to the near-field profiles from different grating and deformation configurations.

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