Refractive index
determination by coherence
scanning interferometry

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Coherence scanning interferometry is established as a powerful noncontact, three-dimensional, metrology technique used to determine accurate surface roughness and topography measurements with subnanometer precision. The helical complex field (HCF) function is a topographically defined helix modulated by the electrical field reflectance, originally developed for the measurement of thin films. An approach to extend the capability of the HCF function to determine the spectral refractive index of a substrate or absorbing film has recently been proposed. In this paper, we confirm this new capability, demonstrating it on surfaces of silicon, gold, and a gold/palladium alloy using silica and zirconia oxide thin films. These refractive index dispersion measurements show good agreement with those obtained by spectroscopic ellipsometry.

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1. INTRODUCTION

The complex refractive index of a material is one of the most important parameters used to design a variety of optical products and optical coatings. Studies to obtain values for the refractive index dispersion started in the early 1950s, and since then, various methodologies have been proposed and developed. Refractive index was conventionally determined by analyzing transmitted and reflected light, using methods such as reflectometry [1] or spectrophotometry [2], but spectroscopic ellipsometry [3], with its advantage of high common-mode rejection, is now the preferred approach. The refractive index is determined by analyzing polarization states of the light reflected from the test sample surface. However, in terms of its metrological capability, this is limited to root mean square interface roughness. In this capacity, coherence scanning interferometry (CSI) [4], previously known as scanning white light interferometry (SWLI), is preferred for the measurement of three-dimensional roughness and topography.

The development of the helical complex field (HCF) function has already been shown to allow the CSI technique to be used for the accurate measurement of thin film thickness [5,6]. The HCF function theory has recently been extended to allow determination of the index of refraction (n) and the extinction coefficient (κ) [7]. Here, we provide an explanation of this new approach using the HCF function together with experimental verification and examples of its application. The CSI technique is capable of providing three-dimensional surface metrology and thin film thickness measurement, but the added capability of determining n and κ on the same sample area is clearly significant. In this paper, the definition of the HCF function differs slightly from that of the original HCF work [6,8]. The Fourier transform exponent polarity is reversed; the resulting HCF function now relates to the mean electrical field reflectance as opposed to its conjugate.

CSI [9,10] is used to measure surface topography based on the height information defined by the location of the interference signal peak. However, additional capabilities of the CSI technique, such as thin film thickness determination, is achieved by analyzing the signal in the frequency domain [8,11] or in the time domain [12]. Methods for obtaining the refractive index with CSI have been previously proposed. Palodhi proposed the polarization-sensitive coherence scanning interferometry (PS-CSI) method [13] by introducing an additional light source and polarizers where high numerical aperture objectives such as ×50 or ×100. Other methods using the phase and power spectrum of the observed interference signals without changing the hardware configuration have also been proposed by S.-W. Kim and G.-H. Kim [14] and de Groot [15]. However, these approaches require large-scale numerical optimization processes in the frequency domain and thus may have a local optimum solution. Mansfield has since found that, through extending the thin film thickness
determination theory based on the HCF function \[6,8\], it is relatively straightforward to determine the refractive index of absorbing thin films or substrates \[7\] because this methodology generates potential refractive index functions prior to optimization. This method has the advantages that no additional hardware is required and complex numerical optimization problem is avoided. This paper presents an evaluation of the HCF-based method for the determination of the spectral refractive index and demonstrates the efficacy of the technique by characterizing three different material substrates.

2. THEORY

The HCF-based method for the determination of the refractive index \[7,16\] is based on the original HCF approach used for film thickness determination \[6,8\]. The method requires two pairs of measurements to be obtained. These are

1. Measurement of the test sample.
   - absorbing film or substrate of unknown spectral refractive index to provide interference signal \(I_1\).
   - a smooth reference substrate with a known refractive index to provide reference signal \(I_{\text{ref}}\).
2. Measurement of the same test sample with a deposited thin film.
   - the same test substrate coated with a thin film of known spectral refractive index to provide interference signal \(I_2\).
   - a smooth reference substrate with a known refractive index to provide reference signal \(I_{\text{ref}}\).

Each measurement pair generates its corresponding HCF function. The first HCF function defines a family of potential spectral solutions. An optimization process then follows in which the second HCF function is sequentially fitted to a synthetic HCF function based on each of the candidate spectral solutions. This establishes the best fit for both the spectral \(n\) and \(\kappa\) potential solutions. This method has the advantages that no additional hardware is required and complex numerical optimization is avoided. This paper presents an evaluation of the HCF-based method for the determination of the refractive index functions prior to optimization. The mean characterization three different material substrates.

A. Reflection from Multilayer Film Assembly

Let the spectral complex refractive index be \(N\), which is a function of the spatial frequency \(\nu\). \(N\) consists of the index of refraction \(n\) and the extinction coefficient \(\kappa\) and is expressed by

\[
N(\nu) = n(\nu) - j\kappa(\nu), \quad \text{where} \quad n, \kappa \geq 0. \tag{1}
\]

The optical admittance is a function of polarization state \((p, s)\), the refractive index \(N\), and the incident angle \(\theta\) for each layer \[17\]

\[
\eta_p = \frac{N\nu}{\cos \theta}, \quad \eta_s = N\nu \cos \theta, \tag{2}
\]

where \(\nu = \{\epsilon_0/\mu_0\}^{1/2}\), and \(\epsilon_0\) and \(\mu_0\) are the permittivity and magnetic permeability of vacuum, respectively. The mean complex reflection coefficient \(r\) of the multilayer film structure, as shown in Fig. 1, (where the \(i\)th layer has thickness \(d_i\), refractive index \(N_{pi}\), and incident angle \(\theta_i\)) is then represented by

\[
r(\nu, d, \theta) = \frac{1}{2}\{r_p(\nu, d, \theta) + r_s(\nu, d, \theta)\},
\]

\[
r_p(\nu, d, \theta) = \frac{\eta_p - Y_{pi}}{\eta_p + Y_{pi}}, \quad \text{where} \quad d = \{d_1, \ldots, d_L\}^T. \tag{3}
\]

Here, \(\eta_{pi}\) and \(\eta_{sub}\) are the optical admittance of the air and the substrate, respectively. \(L\) is the number of layers in the multilayer model and \(Y_{pi}\) is the input optical admittance of assembly for both polarization planes, which is derived from the characteristic matrix of the assembly \([B_{pi}, C_{pi}]\) as follows:

\[
Y_{pi}(d) = \frac{C_{pi}}{B_{pi}}, \quad \text{where} \quad \begin{bmatrix} B_{pi} \\ C_{pi} \end{bmatrix} = I \prod_{i=1}^{L} \begin{bmatrix} -\eta_p \sin \delta_i / \eta_{pi} \\ \cos \delta_i \end{bmatrix} \begin{bmatrix} 1 \\ -\eta_{sub} \end{bmatrix}, \tag{4}
\]

and where

\[
\delta_i = 2\pi\nu N_i d_i \cos \theta_i, \quad \cos \theta_i = 1 - \frac{N_i^2 - \sin^2 \theta}{N_i^2}. \tag{5}
\]

Considering the passage of the incident light through an objective lens, the overall complex reflection coefficient of the layer structure \(r\) is defined by averaging \(r\) over the numerical aperture ranging from \(\theta_{\min}\) to \(\theta_{\max}\) multiplied by the weighting function \(w(\theta)\):

\[
r(\nu, d) = \int_{\theta_{\min}}^{\theta_{\max}} r(\nu, d, \theta) \cdot w(\theta) d\theta,
\]

where

\[
\int_{\theta_{\min}}^{\theta_{\max}} w(\theta) d\theta = 1. \tag{6}
\]

Likewise, the averaged incident angle \(\bar{\theta}\) is also determined as follows:

\[
\bar{\theta} = \int_{\theta_{\min}}^{\theta_{\max}} \theta \cdot w(\theta) d\theta. \tag{7}
\]

The underlying assumption to justify this approach of determining the mean field reflectance is that for a randomly polarized CSI instrument with a low to medium numerical aperture (NA), we regard the \(s\) and \(p\) plane reference mirror (RM) field reflectance to be approximately equal:

\[
r_{RM}(\nu, \theta) \approx r_{pRM}(\nu, \theta). \tag{7}
\]

B. HCF Function

The interference signal \(I(Z)\) along the scanning direction \(Z\) obtained with the CSI instrument consists of a DC component
The presence of transparent films on the substrate distorts the interference signal. Figure 2(b) shows the interference signal from a 560 nm SiO₂ layer deposited on Si substrate. This distortion depends on the layer thickness, the number of thin films, as well as their refractive indices. The CSI instrument used to obtain the signals was a CCI HD (Taylor Hobson Ltd, UK) using a halogen light source.

The HCF function uses this distortion to determine the thin film thickness, where the positive side-band (SB+) of the Fourier transform, denoted by \( \mathcal{F}_{SB+} \), of the interference signals from the film structure and reference sample are used, as shown in Fig. 3. The HCF function is both synthesized and experimentally derived. Let the HCF functions which are given by the actual measurement and theoretically synthesized be \( \text{HCF}^d \) and \( \text{HCF}^r \), respectively. They are expressed by

\[
\text{HCF}^d(\nu) = \tau_{ref}(\nu) \cdot \mathcal{F}\left[ I(\nu)_{SB+} \right],
\]

\[
\text{HCF}^r(\nu, d) = \tau(\nu, d) \cdot \exp\left(\pm j\pi \Delta z_{\text{HCF}} \cos \theta\right),
\]

where the sign of the exponent differs from the original derivation [8] as explained above, where \( I \) is the interference signal intensity, and the unknown parameter \( \Delta z_{\text{HCF}} \) satisfies \(-2\Delta Z_{\text{step}} < \Delta z_{\text{HCF}} < 2\Delta Z_{\text{step}}\). Here \( \Delta Z_{\text{step}} \) is the data-sampling interval of the interference signal which is normally about from 60 to 70 nm taking account of the Nyquist frequency depending on the type of the light source used in the measurement.

Denoting the reference by the subscript ref, \( \tau_{ref} \) represents the amplitude reflection coefficient and \( I_{ref} \) is the interference signal. The key attribute of the reference sample is that it has a well-known spectral refractive index. In addition, it needs to be polished and reasonably flat to provide specular reflection. Normally, a reflective sample such as Si or B270 (SCHOTT Glass) is used. Through common-mode rejection, the reference measurement allows potential errors such as a slowly varying light source to be compensated.

As an aside, when Mansfield coined the term HCF for this function [6, 8] he was unaware of the earlier related work of Kim and Kim [11] and de Groot and de Lega [12]. Inspection of Eq. (8) regarding the synthetic HCF shows that the real and imaginary components of the exponent generate a helix in frequency space, while the mean reflected electrical field term distorts this both in terms of phase and amplitude.

The distortion of the signal due to the thin film is translated into phase and amplitude in the frequency domain and the HCF method uses this information to determine the film thickness. As an example, Fig. 3 shows the amplitudes of the Fourier transform of the signals from a bare Si substrate and an SiO₂ film deposited on the Si substrate corresponding to Figs. 2(a) and 2(b), respectively. As is well known, if \( a(\nu) \) is the transform of a real function, then there is a conjugate relationship between the positive and negative frequencies, \( a(-\nu) = a^*(\nu) \). The \( \text{HCF}^d \) function uses the positive side-band, denoted by SB+, as shown in Fig. 3.

The set of the film thicknesses \( d \) is dispersively determined by minimizing the least squared error function \( J_{\text{HCF}} \) in Eq. (9) with respect to \( d \) and \( \Delta z_{\text{HCF}} \). The result of such error-minimization yields the best-fitting synthetic HCF. Figure 4 shows the real and imaginary components of both HCF and \( \text{HCF}^d \). The problem can be stated as

\[
\min_{\Delta z_{\text{HCF}}, d} J_{\text{HCF}} = \int_{\nu} \left| \text{HCF}^d(\nu) - \text{HCF}^r(\nu, d) \right|^2 \, d\nu
\]

subject to \(-2\Delta Z_{\text{step}} < \Delta z_{\text{HCF}} < 2\Delta Z_{\text{step}}\) (9)

where a conjugate gradient method is used to evaluate the merit function \( J_{\text{HCF}} \).

C. Refractive Index Determination Using the HCF Function

This method requires that the objective lens has a low or medium numerical aperture (NA). However, if a low NA objective is used such that field variations over the NA may be reasonably ignored, then the analysis is much more straightforward.
Now, given that unknown refractive index as $\hat{N}$ to potential solutions together with its synthetic equivalent are described by $\text{HCF}$ designated $z$. Each measurement requires two pairs of measurements. These correspond to two measurement pairs to be the same. In this case, the required family of potential spectral $n$ and $\kappa$ solutions may be generated analytically [7]. The refractive index of the test sample can be numerically determined from the HCF function when signals from two material structures are provided. The unknown test sample and the known thin film deposited on the test sample are shown schematically in Fig. 5. The subscripts of 1 and 2 are given the known thin film deposited on the test sample are shown schematically in Fig. 5. Each measurement pair generates its corresponding HCF function, designated $\text{HCF}^i (\nu)$, where $i$ is 1 or 2.

Starting with the first HCF function, if the test sample has a refractive index $N_f (\nu)$, then the corresponding HCF function together with its synthetic equivalent are described by

$$\text{HCF}_1^d (\nu) = r_{ref} (\nu) \cdot \frac{\mathcal{F}[I_1(Z)]_{SB+}}{\mathcal{F}[I_{ref}(Z)]_{SB+}},$$

$$\text{HCF}_1^i (\nu, 0) = \frac{1 - N_f (\nu)}{1 + N_f (\nu)} \cdot \exp (+ j \pi \nu \Delta z_{\text{HCF}1}),$$

where $-2 \Delta Z_{\text{step}} < \Delta z_{\text{HCF}1} < 2 \Delta Z_{\text{step}}$. (10)

Now, given that $\text{HCF}_1^d = \text{HCF}_1^i$, we can generate a family of potential solutions $\hat{N}$ as a function of $\Delta z_{\text{HCF}1}$ for the unknown refractive index as

$$\hat{N}_f (\nu, \Delta z_{\text{HCF}1}) = \frac{\exp (+ j \pi \nu \Delta z_{\text{HCF}1}) - \text{HCF}_1^d}{\exp (+ j \pi \nu \Delta z_{\text{HCF}1}) + \text{HCF}_1^i},$$

where $-2 \Delta Z_{\text{step}} < \Delta z_{\text{HCF}1} < 2 \Delta Z_{\text{step}}$. (11)

For example, the candidate solutions $\hat{N}$ for a gold test substrate are shown in Fig. 6 together with the true refractive index determined by spectroscopic ellipsometry.

Now considering the second HCF function, referring to Fig. 5 the coated sample has a film of physical thickness $d$ and known index $N_f (\nu)$. The corresponding HCF function together with its synthetic equivalent are described by

$$\text{HCF}_2^d (\nu) = r_{ref} (\nu) \cdot \frac{\mathcal{F}[I_2(Z)]_{SB+}}{\mathcal{F}[I_{ref}(Z)]_{SB+}},$$

$$\text{HCF}_2^i (\nu, d | \hat{N}) = r_2 (\nu, d | N_f, \hat{N}) \cdot \exp (+ j \pi \nu \Delta z_{\text{HCF}2}),$$

where $-2 \Delta Z_{\text{step}} < \Delta z_{\text{HCF}2} < 2 \Delta Z_{\text{step}}$. (12)

The field reflectance term $r_2$ is evaluated using Eq. (3). Also, there is no requirement for the reference samples used for the two measurement pairs to be the same.

The solution to Eq. (11) may be expressed by the requirement

$$\min \int |\text{HCF}_2^i (\nu) - \text{HCF}_2^i (\nu, d | \hat{N})|^2 d\nu$$

subject to $-2 \Delta Z_{\text{step}} < \Delta z_{\text{HCF}1} < 2 \Delta Z_{\text{step}}$. (13)

In practice, initially a family of $\hat{N}_f (\nu, \Delta z_{\text{HCF}1})$ spectral $n$ and $\kappa$ candidates (typically ~25, although ~50 in the case of gold) are generated using Eq. (11). These correspond to $\Delta z_{\text{HCF}1}$ ranging over $\pm 2 \Delta Z_{\text{step}}$. Next, in a sequential manner, running through all the candidate solutions, $\int$ is minimized. In fact, these conjugate gradient-based individual optimizations are identical to the standard HCF fitting for a single layer, given that there are two unknowns, $d$ and $\Delta z_{\text{HCF}2}$. Finally, the value of the merit function with respect to $\Delta z_{\text{HCF}1}$ is locally quadratically interpolated to determine the optimum value for $\Delta z_{\text{HCF}1}$. Application of
Eq. (11) yields the refractive index \( N_i = n_i - j\kappa_i \) of the test sample.

3. EXPERIMENT

A. Experimental Setup

All the transparent SiO\(_2\) and ZrO\(_2\) films were deposited using pulsed DC magnetron sputtering in a reactive process. The substrates were mounted vertically on a carrier rotating at \( \sim 100 \) rpm to provide horizontal uniformity. A trimming mask was placed in front of the magnetrons to achieve uniformity in the vertical direction. Overall, thin film thickness uniformity was better than \( \pm 2\% \) for films deposited over an area of \( 60 \) mm \( \times \) 60 mm for film thickness greater than \( \sim 50 \) nm.

The CSI instrument used to obtain the interference signals was a CCI HD fitted with a halogen light source; configured as such, it exhibits a mean wavelength. This instrument features the halogen light source with a 631 nm average wavelength, and it is shown in Table 1 [18]. Analysis of the interference signals were conducted after the measurements using the software written in MATLAB (The MathWorks, Inc).

For comparative study of the refractive indices, the spectroscopic ellipsometer (UVISEL iHR320FGAS provided by Horiba Jobin Yvon) was used. The refractive indices together with the film thicknesses were determined by the software program attached with this system.

B. Measurement Condition

Four measurements were conducted on the three different materials, as shown in Tables 2 and 3. A Si substrate was used as a reference material to obtain the reference signal \( I_{ref} \). The experimental conditions used to deposit the metal-oxide thin films have been previously reported [5].

C. Refractive Index Determination and Analysis

Figures 7–10 illustrate comparative spectral plots of the refractive indices determined by the HCF-function-based method and by spectroscopic ellipsometry on the test samples given in Table 2. The error bars represent the sample standard deviation over the number of the measurements shown in Table 3.

All the refractive indices in Figs. 7–10 determined by this HCF-based method show reasonable fits with those of spectroscopic ellipsometry. In particular, the extinction coefficients \( \kappa \) of the gold sample exactly correspond to each other in the broad wavelength range. All of the results exhibit a high frequency jitter. The signal-to-noise ratio is best in the mid-visible range. As the limits of the bandwidth (430–730 nm) are approached, there is a deterioration in the signal/noise. However, the most likely source for such jitter is the presence of very small scanning nonlinearities.

Table 3 shows the root mean square (RMS) error between the refractive indices obtained by the HCF-based method and by spectroscopic ellipsometry together with the corresponding 550 nm refractive index ratio; this ratio indicates how critical the RMS errors are at 550 nm. Table 5 shows the correlation coefficients between the refractive indices determined by the HCF-based method and spectroscopic ellipsometry; the shape similarity of the spectral profiles of the refractive indices is characterized by these coefficients. As evident from Tables 4 and 5, the gold sample refractive indices are a very close match both in terms of spectral trend and absolute value deviation; on the
other hand, the #1 Si sample exhibits a relatively mediocre match in terms of spectral trend and a significantly larger absolute value deviation.

4. DISCUSSION

The exact determination of $\Delta z_{\text{HCF1}}$ plays an important role in this method. In order to understand the sensitivity of the refractive index with respect to $\Delta z_{\text{HCF1}}$, absolute values of partial derivatives of the index for samples #2 and #3 have been investigated. The partial derivatives of the candidates for the refractive index are, from Eq. (11),

$$\frac{\partial N_t}{\partial \Delta z_{\text{HCF1}}} = \text{Re} \left\{ \frac{\pi \nu \cdot \text{HCF} \cdot \exp (+j4\pi \nu \Delta z_{\text{HCF1}})}{\{\exp (+j4\pi \nu \Delta z_{\text{HCF1}}) + \text{HCF}\}^2} \right\}$$ (14)

Figures 11 and 12 demonstrate the variability of this partial derivative. Optionally, it may be used to weight the synthetic $\Delta z_{\text{HCF1}}$ so as to provide nominally equi-spaced $N_t$ solutions instead of equi-spaced $\Delta z_{\text{HCF1}}$ samples. The relatively large standard deviation at longer wavelengths apparent in Fig. 9 is probably due to the large absolute value of the partial derivative of the refractive index, as shown in Fig. 12, whereas the relatively stable standard deviation seen in Figs. 8 or 7 is probably due to the relatively constant partial derivative, as shown.

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Table 4. Root Mean Square Error between $n$ and $\kappa$ Determined by the HCF Method and Spectroscopic Ellipsometry in the Bandwidth (430 to 730 nm) and Their Ratios to Representative $n$ and $\kappa$ at 550 nm Wavelength, the Best Values are Emphasized

<table>
<thead>
<tr>
<th>Sample #</th>
<th>RMS Error$^a$</th>
<th>Ratio to $n$ and $\kappa$ 550 nm$^b$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$(n, \kappa)$ at 550 nm</td>
<td>$n$</td>
</tr>
<tr>
<td>#1 (4.12,0.42)</td>
<td>0.016</td>
<td>0.032</td>
</tr>
<tr>
<td>#2 (4.14,0.30)</td>
<td>0.013</td>
<td>0.007</td>
</tr>
<tr>
<td>#3 (0.39,2.46)</td>
<td>0.012</td>
<td>0.006</td>
</tr>
<tr>
<td>#4 (1.63,2.87)</td>
<td>0.034</td>
<td>0.038</td>
</tr>
</tbody>
</table>

$^a$The number of data points is 120 ranging from 430 to 730 nm.

$^b$(RMS error)/(n or $\kappa$) at 550 nm wavelength, respectively.

Table 5. Correlation Coefficients between $n$ and $\kappa$ Determined by the HCF Method and Spectroscopic Ellipsometry, the Best Values are Emphasized

<table>
<thead>
<tr>
<th>Sample #</th>
<th>Correlation Coefficient (%)$^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$n$</td>
</tr>
<tr>
<td>#1</td>
<td>97.9 ± 0.7</td>
</tr>
<tr>
<td>#2</td>
<td>93.6 ± 2.2</td>
</tr>
<tr>
<td>#3</td>
<td>97.3 ± 0.9</td>
</tr>
<tr>
<td>#4</td>
<td>72.5 ± 8.4</td>
</tr>
</tbody>
</table>

$^*$The confidence interval is 95%.
in Fig. 11. Returning to the results in Figs. 7–10, the merit function associated with Fig. 7 exhibits a particularly flat bottom; as a consequence, to ensure stability, for this substrate/film pairing the original merit function was replaced by one based on symmetry. In Fig. 9, the bumpiness exhibited by the determined \( n \) and \( \kappa \) is due to the presence of small \( z \)-scan errors. This would be expected to improve if a larger number of measurements were used. Figure 9 shows essentially excellent agreement, while the offsets apparent in Fig. 10 in both \( n \) and \( \kappa \) are consistent with external vibrations present when the one reference measurement was taken.

The sensitivity clearly improves as the film-index-dependent merit function minimum becomes better defined; for the Si substrate, the difference in particular determined using SiO\(_2\) and ZrO\(_2\) deposited films is apparent.

5. CONCLUSION

CSI is a well-established technique for surface topography, and the introduction of various approaches including the HCF function to CSI extended this capability to cover thin film thickness determination. Together with experimental verification, this paper presents an expose of a proposed further extension of the HCF function to the refractive index determination of substrates or absorbing films. CSI together with the HCF function has an advantage over spectroscopic ellipsometry in that it is able to provide both surface and subsurface boundary topography. One benefit of this approach for refractive index determination is that no additional hardware is required; the computation is a reasonably straightforward extension to that used for thin film determination. The comparative spectral plots of the refractive indices and extinction coefficients show good agreement, thereby verifying this approach. The determined refractive index stability can be influenced by the sensitivity of the refractive index regarding the numerical optimization. Additionally, the spectral refractive index sensitivity is dependent on the index of the deposited film. It is acknowledged that this approach places significant demands on the CSI scanning \( z \) stage; this most realistic way of improving this aspect of spectral refractive index \( (n \) and \( \kappa \) determination is simply through taking more repeat interference measurements.

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