

Theoretical and experimental investigation of phase singularities generated by optical micro- and nano-structures

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Abstract

Phase singularities appear in the diffracted far-field of an optical micro-structure if the object is of a sufficient lateral size to induce an appropriate phase delay. We present results that determine the critical dimension of a single phase bar for the generation of dislocations in the far-field. Using scalar theory, an analytical equality is derived that must be met by the structure. Because the size of the object is comparable to the theory is used to find this feature size for a wavelength, rigorous diffraction true object. Once the dislocations appear, their position is related strongly to the geometry of the object. We show theoretically and experimentally by using an interference microscope that, for a single phase bar, the distance between pairwise generated dislocations depends, to a good approximation, linearly on the width of the structure.

Keywords: phase singularities, high-resolution microscopy, diffraction

1. Introduction

Phase singularities are points in space where the real as well as the imaginary part of an electromagnetic field becomes zero and consequently the phase cannot be determined [1]. The phase jumps always by π while scanning through a dislocation, independent of the scan direction. The gradient of the phase becomes infinite at this position and the phase variation along a closed loop around such a point is always an integer multiple of 2π , the topological charge of the vortex [2]. Illuminating optical micro- and nano-structures with an arbitrary wavefield might induce a scattered field that interferes entirely destructively with the illuminating wavefield, thus creating a phase singularity at this point [3–5]. The position and consequently the relative distance

between these pairwise generated dislocations can be linked to the geometry of the structure [6]. Because the accuracy of the determination of the position for dislocations is not restricted by the classical diffraction limit, the geometry of the object can be determined with a high accuracy by using *a priori* information about the object, which offers a valuable tool for metrological applications [7, 8]. An example of this is the semiconductor industry, where it is necessary to measure the lateral dimensions of structures using non-destructive techniques, the distances between phase singularities providing a high precision quality factor for fabricated objects. A more general application is the calibration of length standards on a sub-micron length scale.

The instrument we are using for the interferometric measurements functions in transmission: hence we will restrict our investigations to the case where the object that

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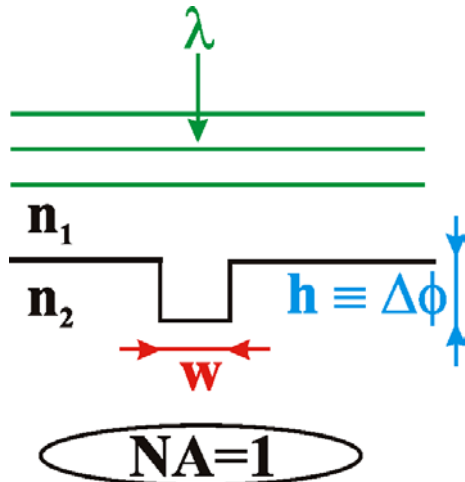


Figure 1. Basic set-up of the problem under investigation.

generates the scattered field works likewise in transmission and has a refractive index that is comparable to most glasses and polymers. Additionally, the instrument is, in principle, a classical microscope and has no access to the evanescent part of the angular spectrum of the transmitted wave field, due to the numerical aperture being equal to or smaller than 1. This low-pass filtering property will be taken into account for all the calculations to compare theory with measurement. The field that is measurable in the high resolution interference microscope (HRIM) is essentially a paraxial field that has no longitudinal component. We will discriminate in this two-dimensional problem the two cases where the field is TE-polarized (the vector of the electric field oscillates parallel to the space-invariant direction of the structure) and TM-polarized (the vector of the magnetic field oscillates parallel to the space-invariant direction of the structure) and analyse the position of the singularity in the electric field for TE polarization and the position of the singularity in the magnetic field for TM polarization. Nevertheless, both coincide in the paraxial approximation that holds for the measurements.

Figure 1 shows the basic geometry of the problem considered in this paper. Two half-spaces with different refractive indices n_1 and n_2 are separated by a planar surface. The illuminating wavefield with wavelength λ is a planar wave. The half-spaces are perturbed by a phase bar that is a trench within the plane surface. The parameters of the trench are its width w and its geometrical height h . The optical height is given by $\Delta\phi = k(n_2 - n_1)h$ with k being the wavenumber. If the phase bar is much smaller than the wavelength, it will not interact with the incoming wavefront efficiently and, as a consequence, the transmitted field is comparable to a plane wave. Increasing the dimension of the object will lead to a more pronounced scattered field and from a certain dimension on the scattered field will interfere with the incident wavefield such that complete destructive interference gives a point in the second half-space where a phase dislocation appears.

In this paper we will investigate the object conditions necessary for the generation of phase singularities in the far-field and the subsequent spatial dependence as a function of the geometry of the object.

In section 2 we will determine the smallest size of an object that can generate a phase singularity in the far-field. This

will be done using scalar theory as well as by using an exact rigorous diffraction theory. The choice of a proper polarization for the illuminating wavefield as well as the variation of the distance between singularities by changing the object width is discussed. In section 3 we analyse experimentally the variation of this distance as a function of the width of the object. For this purpose we present the experimental set-up of the HRIM and analyse its accuracy for the measurement of the distance between phase singularities.

2. Conditions for the generation of singularities

2.1. Scalar approximation

For the derivation of the condition for the appearance of a phase singularity in the diffracted far-field of an optical microstructure, we will start for simplicity at the condition for a grating. The far-field of such an object is written as a superposition of a discrete number of plane waves, which have an amplitude a_m . A singularity appears only if the sum over all propagating amplitudes except the highest amplitude is equal to the highest amplitude. Otherwise a complete destructive interference is not possible. This condition is as [9]

$$\sum_{m \neq n} |a_m| \geq |a_n| \quad \forall n, \quad (1)$$

where the sum is taken over all the amplitudes that propagate. The proof of equation (1) is given in the appendix. For the problem of finding the dimensions of a perturbation such that a singularity is generated, we assume that the highest amplitude is always the amplitude of the zero-order because in the unperturbed case this is the only order that has a value which differs from zero. Introducing a perturbation will couple light into other orders but the order with the highest amplitude will be always the zero-order before a singularity is generated, hence $a_n = a_0$. In the paraxial approximation the strength of the diffracting amplitudes is calculated by doing a Fourier transformation of the transmission function $T(x)$ of the object [10] that relates the field behind the structure $U_{\text{Trans}}(x)$ to the illuminating field $U_{\text{Inc}}(x)$ by a simple multiplication $U_{\text{Trans}}(x) = T(x)U_{\text{Inc}}(x)$. For the treatment of single objects we calculate the amplitude for the limit of an infinite period. The summation over the discrete spectrum of plane waves in equation (1) will become an integration over a continuous spectrum of the propagating part of the spectrum. This gives

$$\int_{\nu} |a(\nu)|(1 - \delta(\nu - \nu_0)) d\nu \geq \int_{\nu} |a(\nu)|\delta(\nu - \nu_0) d\nu$$

$$\Lambda \rightarrow \infty. \quad (2)$$

Using the transmission function of a single phase bar

$$T(x) = \begin{cases} e^{i\frac{2\pi h}{\lambda}(n-1)} & |x| \leq \frac{w}{2} \\ 1 & |x| > \frac{w}{2} \end{cases} \quad (3)$$

and calculating the Fourier transformation we derive the equality

$$0 = 1 - \frac{4}{\pi} \sin\left(\frac{\Delta\phi}{2}\right) \int_0^{\pi w} \frac{|\sin(\frac{t}{\lambda})|}{t} dt$$

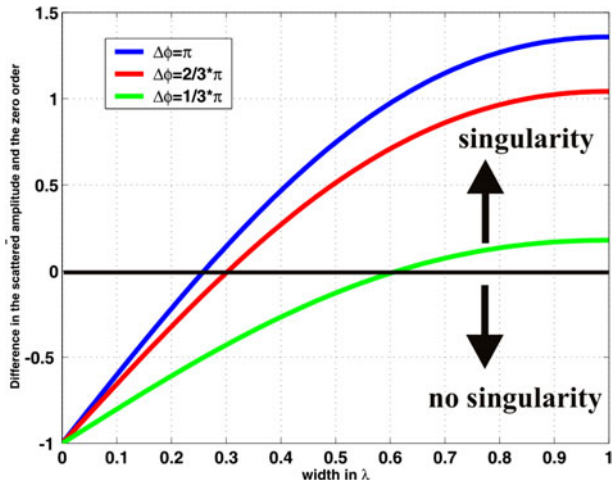


Figure 2. Evaluation of equation (4) for three different phase values.

that must be fulfilled by the structure in order to generate a phase singularity in the far-field. The equation is derived in the appendix. The integral cannot be solved analytically and further simplification is not possible. Figure 2 shows the numerically evaluated difference between the right- and left-hand sides of equation (4) as a function of the width of the phase bar in units of the wavelength for three different induced phase delays. For a cooperative scatterer, that is an object which induces the maximum possible phase delay of π , the smallest width of a phase bar that generates a singularity in the far-field is $\lambda/4$. Smaller structures will not induce a sufficiently strong scattered field. If the induced phase delay is smaller than π , the width of the structure has to be consequently larger for the generation of a phase singularity. If the phase delay is, for example, $\frac{2}{3}\pi$, the width must be approximately 0.3λ , and in the case of an induced phase delay of $\frac{1}{3}\pi$ the width must be 0.6λ . The condition for the appearance of dislocations generated by arbitrary objects can be found using equation (2) and applying the same procedure as described in the appendix for the phase bar. In cases where the transmission spectrum cannot be found analytically, simple numerical routines can be used to evaluate the integrals. As a second example for the application of the proposed criteria in equation (2), we show in figure 3 the smallest width of two phase bars as a function of the separation such that they generate a dislocation in the far-field. The induced phase delay of both bars is π . If they are not separated, the width corresponds to half of the width of the single bar that generates a dislocation. Increasing the distance will decouple them. For separation distances larger than the wavelength, the bars behave like a Fabry–Perot resonator and an oscillating behaviour can be seen, which is attributed to a scattered field that suffers from back and forth reflections between the structures.

All the feature sizes for the objects which can generate a phase singularity in the far-field are comparable to the wavelength. In this region, the scalar and paraxial approximations no longer hold and one has to use a rigorous diffraction theory to describe properly the interaction of a light wave with such a structure. Consequently we will use a grating theory [11] to predict the smallest size of a real object that can generate a singularity in the far-field without

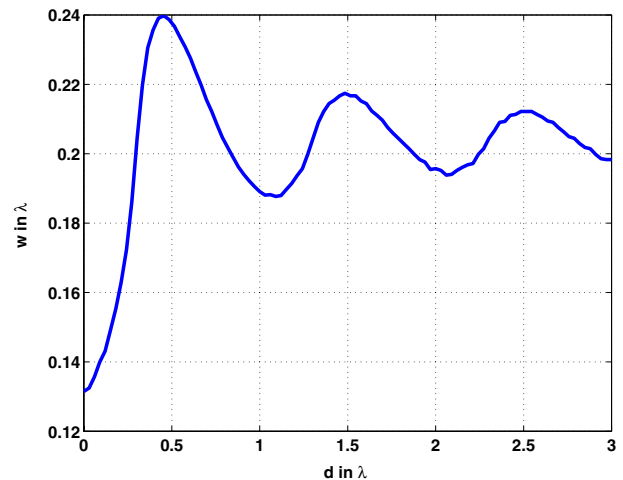


Figure 3. Width of two π -phase bars for which a dislocation appears as a function of the distance between the two bars.

any approximation. Such a grating theory can be used for the modelling of single objects by choosing a sufficiently large period in the calculation, which is additionally not an integer multiple of the period.

2.2. Rigorous treatment

By using rigorous diffraction theory, we have to choose the polarization of the illuminating wavefield. We will use a TM-polarized wave because it is known that, for the current structure, a phase singularity appears at smaller feature sizes for this polarization. The trench can be regarded as a waveguide. If the material would be a perfect conductor, a cut-off width would exist for TE polarization. For structures smaller than this width no mode is excited and the field cannot penetrate the structure. On the other hand, for TM polarization a mode can always be excited. For the present geometry the same arguments can be applied. For TE polarization no mode is efficiently excited and hence the field scattered by the defect will not be strong enough to perturb the transmitted plane wave sufficiently. For TM polarization such a mode is excited and will generate a sufficiently strong scattered field, which can interfere completely destructively with the transmitted plane wave to create a singularity. Hence we use a TM-polarized plane wave to generate a phase singularity at a feature size that is as small as possible [12].

Figure 4 shows the distance between a pair of generated singularities directly behind the structure as a function of the width of the object if the induced geometrical phase delay is π . As the illuminating wavelength we have used 488 nm, the refractive index of the medium in the first half-space was 1, the refractive index of the medium in the second half-space was 1.5 and the geometrical height was chosen consequently equal to the wavelength.

For the determination of the distance between the phase singularities, we have calculated first the complex field distribution directly behind the trench for each width using the rigorous coupled wave analysis (RCWA) [11]. RCWA is a grating theory that can be applied to the description of single objects by choosing a period much larger than the wavelength and not an integer multiple of the wavelength.

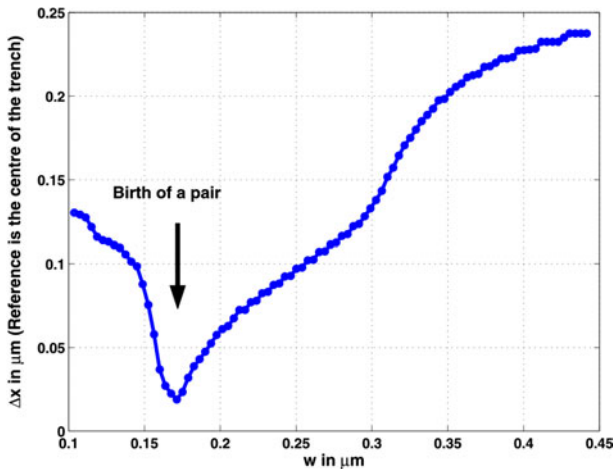


Figure 4. Distance between singularities generated behind a trench as a function of its width.

We have used a period of $20.2 \mu\text{m}$ in the calculation and the number of diffraction orders that were retained in the plane wave expansion was sufficiently large such that the position of the singularities converges to a fixed value.

Before determining the position of the phase singularity we have low-pass-filtered the field distributions assuming a numerical aperture equal to unity.

For the determination of the position of the dislocations we have calculated the gradient of the locally unwrapped phase distribution. The gradient of the phase in a singularity is infinity. Describing the fields numerically will not give infinite values for the gradient, but finding the maximum of the gradient and applying a simple threshold criteria determines the position of the dislocations automatically without ambiguity and with a sufficiently high precision. To find out whether the point in the field with the highest phase gradient corresponds to a phase singularity or not, we have used an algorithm for the detection of a singularity described in the literature [13].

From figure 4 and from the corresponding field distributions that were calculated, we deduce a phase bar with a width of 180 nm as the smallest width of an object that generates a phase singularity in the far-field. The points in figure 4 for phase bars with a smaller width are not the distance between the singularities but rather the distance between the points with the highest phase gradient. The width of 180 nm is higher than the predicted scalar value of 122 nm . This is not a surprise because, by treating the problem rigorously, we see that light is already diffracted inside the structure, which will lead to transport of energy away from the trench while passing through the structure. The field is somewhat smeared out and the sharp character of the field distribution assumed in the thin element approach is lost. Additionally, the phase delay induced by such a structure is, for the same reason, always weaker and hence smaller than π [14]. Consequently the phase singularity for real objects will appear at feature sizes larger than the predicted scalar value. Nevertheless, increasing the contrast in the refractive index between the first and the second half-space allows the appearance of phase singularities for smaller objects.

Additionally, it can be seen from figure 4 that the distance between the singularities scales, to a good approximation,

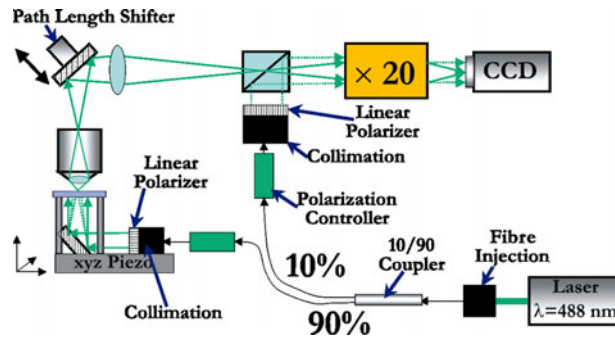


Figure 5. Geometrical set-up of the high resolution interference microscope.

linearly with the width of the trench. Because the phase singularities can be measured with a very high precision, topological features of the structure can be similarly determined with a high resolution, assuming that *a priori* knowledge about the object is available. In the next section we will show experimental results on the behaviour of phase singularities generated by a trench written in photoresist using an electron beam.

3. Measurements with the HRIM

Figure 5 shows the experimental set-up of the HRIM. An argon laser ($\lambda = 488 \text{ nm}$) is used as a light source and the interference microscope consists of a reference arm and a signal arm. Two essentially telescopic magnification stages lead to a magnification of approximately 1000 that gives access to the relevant nanometric lateral scale. A pixel of the CCD camera corresponds, after calibration with a grating, to 20 nm in the object plane. The object is located on a x - y - z piezo stage. The z axis allows successive movement in the third dimension, that makes it possible to measure the field along the propagation direction. The phase distribution is determined by a classical five-frame interference algorithm in each z plane and a subsequent phase reconstruction algorithm that assumes a plane wave distribution far away from the scatterer gives the relative phase along the z direction. Because the trenches are grooves running in the y direction, the field is invariant along this direction too. For a reduction of the noise the measured fields are averaged in the y direction. The numerical aperture of the system is 0.85. Figure 6 shows the measured intensity and phase (isophases) distribution behind a trench and in figure 7 the rigorously simulated intensity and phase distribution is shown.

Please note that the transition goes from photoresist (top) to air (bottom) and in the figure the illumination direction is along the z direction from the top. As the refractive index we have assumed 1.5, the width was 450 nm and the height was 450 nm . As for the illumination wavefield it was TM-polarized. An overall excellent agreement between calculation and measurement can be seen. The two characteristic singularities appear directly behind the structure and are indicated by circles. These are the singularities that can be related to the width of the object. Four additional singularities appear in the measured as well as in the simulated virtual field in front of the structure. This is a virtual field because it actually

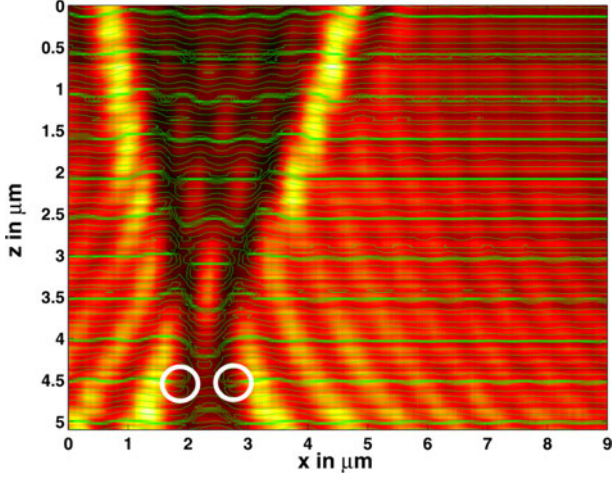


Figure 6. Measured intensity and phase distribution in the far-field of a single trench in photoresist ($w \approx 0.5 \mu\text{m}$).

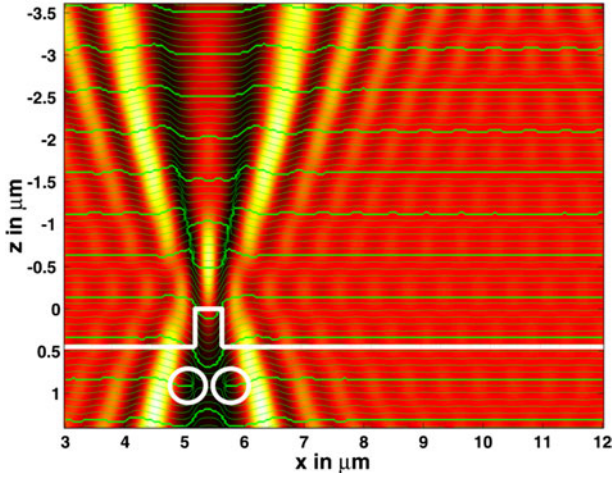


Figure 7. Calculated intensity and phase distribution in the far-field of a single trench in photoresist ($w = 0.45 \mu\text{m}$, $h = 0.45 \mu\text{m}$).

results from the back-propagated transmitted field distribution in the first half-space. To determine the reproducibility of our instrument we determined the distance between dislocations of the same structure several times. We found an accuracy of 3 pixels for the CCD camera, that corresponds to a resolution of 60 nm.

To verify experimentally the linear behaviour of the distance between singularities and the width of the phase bar, we fabricated a series of trenches with an increasing linewidth. Figure 8 shows the results. The trench width difference between two measurements alternates between 20 and 30 nm and the largest trench was 500 nm. The theoretically predicted linear behaviour can be seen. In our measurements the smallest structure that can generate a singularity in the far-field is a trench width of 360 nm. The field distribution of smaller trenches was measured but no singularity appears in the diffracted far-field. This width is higher than the predicted value in section 2 due to the smaller numerical aperture. An additional source for the deviation from the optimum value is the non-optimal height which cannot be controlled with the desired precision. Additionally, the refractive index of the photoresist is subject to ambiguities. Nonetheless, the

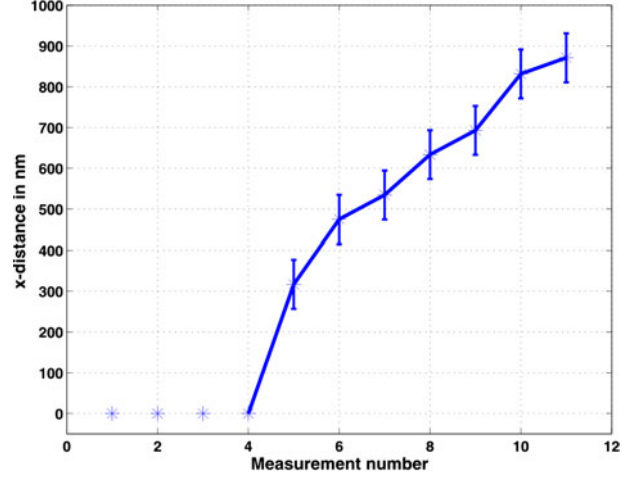


Figure 8. Measured x distances between dislocations generated by a trench with increasing width.

principal behaviour is comparable to the theoretically predicted one.

4. Conclusions

We have shown theoretically and experimentally that there is a minimum lateral feature size for an object for the generation of a singularity in the far-field of the structure. In the scalar approximation this smallest feature size is $\lambda/4$ and thus comparable to the diffraction limit. For the class of objects in the present investigation the real size for the object using a rigorous calculation is somewhat higher. Once the singularity pairs appear, their separation is, to a good approximation, linear with the width of the object. The linear dependence has been proved experimentally using a HRIM, with a spatial resolution for the distance determination of approximately 60 nm.

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Appendix

The field behind a grating, written as a superposition of plane waves, is given by

$$U(\mathbf{r}) = \sum_m a_m e^{i\mathbf{k}_m \mathbf{r}}. \quad (\text{A.1})$$

A phase singularity appears if the field is zero: hence

$$\sum_m a_m e^{i\mathbf{k}_m \mathbf{r}} = 0. \quad (\text{A.2})$$

Subtracting an arbitrary order a_n from both sides of equation (A.1) gives [9]

$$\sum_{m \neq n} a_m e^{i\mathbf{k}_m \mathbf{r}} = -a_n e^{i\mathbf{k}_n \mathbf{r}}. \quad (\text{A.3})$$

Taking the absolute value

$$\left| \sum_{m \neq n} a_m e^{i \mathbf{k}_m \mathbf{r}} \right| = |-a_n e^{i \mathbf{k}_n \mathbf{r}}| = |a_n| \quad (\text{A.4})$$

and applying the triangular inequality finally leads to

$$\sum_{m \neq n} |a_m| \geq |a_n|, \quad (\text{A.5})$$

which is equation (1) [9].

For the binary phase grating whose transmission function is given by

$$T(x) = \begin{cases} e^{i \frac{2\pi h}{\lambda} (n_1 - n_2)} & 0 \leq x < w \\ 1 & w \leq x < \Lambda \end{cases} \quad (\text{A.6})$$

the amplitude of the m th order upon plane wave illumination is given by [10]

$$a_m = \frac{1}{\Lambda} \left[\int_0^w e^{i \Delta \phi} e^{-i m \frac{2\pi}{\Lambda} x} dx + \int_w^\Lambda e^{-i m \frac{2\pi}{\Lambda} x} dx \right] \quad (\text{A.7})$$

with $\Delta \phi = \frac{2\pi}{\lambda} (n_2 - n_1) h$. By solving the integral we find the absolute value of the m th amplitude as

$$|a_m| = \frac{2}{\pi} \sin \left(\frac{\Delta \phi}{2} \right) \frac{|\sin(\frac{m\pi w}{\Lambda})|}{|m|}. \quad (\text{A.8})$$

The sum of all propagating orders is

$$\sum_m |a_m| = \frac{4}{\pi} \sin \left(\frac{\Delta \phi}{2} \right) \sum_{m=1}^{\frac{\Lambda}{\lambda}} \frac{|\sin(m \frac{\pi}{\Lambda} w)|}{m}. \quad (\text{A.9})$$

In the limit of an infinite period the amplitude of the zero-order is unity and the scattered field is

$$\begin{aligned} & \int_v |a(v)| (1 - \delta(v - v_0)) dv \\ &= \frac{4}{\pi} \sin \left(\frac{\Delta \phi}{2} \right) \int_0^{\pi w} \frac{|\sin(\frac{t}{\lambda})|}{t} dt. \end{aligned} \quad (\text{A.10})$$

A phase singularity appears if the integral over the scattered amplitudes equals the zero amplitude, which is equation (4).

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