Theory of speckles in diffractive optics and its application to beam shaping

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Abstract

The paper considers the design of diffractive phase elements (DPEs) for solving the general beam shaping problem where the signal wave is specified by an intensity distribution on a continuous support in a finite signal window. In this case serious design problems due to speckles may arise.

After introducing a mathematical definition and description of speckles, the influence of the phase of the signal wave on the design process is examined. It turns out that depending on the application a pseudo-random or a spherical phase should be used as an initial phase of the signal wave for an iterative design procedure.

Due to its smoothness the spherical phase prevents the occurrence of speckles during the iteration process whereas the pseudo-random phase is accompanied by speckle effects. For applications where the imaging properties of the spherical phase are undesirable a soft coding method is presented which significantly reduces the number of speckles of the pseudo-random phase. For cases where speckles still remain we finally present an approach for removing these in pairs.

1 Introduction

Beam shaping with diffractive elements is of great importance in various laser applications such as material processing, proximity printing or pattern projection. In literature beam shaping usually means the transformation of a laser beam, e.g. a Gaussian beam, into a beam of different shape. From a general point of view beam shaping is the transformation of a specified illumination wave into a specified diffracted wave—referred to as the signal wave in the following—by an optical component. When applying scalar diffraction theory, both the illumination wave and the signal wave can be described by complex-valued functions defined on a continuous support.

Methods of diffractive optics can be successfully applied in the design of diffractive elements (DEs) solving beam shaping problems. The computeraided design of DEs offers a maximum in flexibility to find a transmission function fulfilling the specifications posed by the application. In some cases analytical solutions based on geometrical optics can be derived by applying the method of stationary phase [1] to find the transmission function of a DE [2, 3] performing the desired wave transformation. However, we will consider general beam shaping problems for which no analytical solutions exist. In this case, well-known design algorithms such as iterative fourier transform algorithms (IFTAs) [4, 5, 6], direct binary search (DBS) [7] and simulated annealing (SA) [5] can be used to compute a transmission function fulfilling the problem specification.

Some applications require the generation of a signal wave with a complex amplitude specified in a finite domain referred to as the signal window W_{Signal} . An algorithm for the design of a DE solving the beam shaping problem is described in [8]. However, there are many applications where only the intensity of the signal wave is of interest. In this case the signal phase is a parameter of freedom that can be used in the design of a DE to fulfil constraints imposed on the signal wave and the transmission function of the DE. Thus, the quality of the intensity profile of the signal wave as well as the diffraction efficiency of the DE may be considerably improved. This paper considers the general beam shaping problem under the assumption that the signal phase can be used as a free parameter in the DE design. In applications in which a certain signal phase is required a second DE correcting the signal phase could be introduced.

In the iterative design a serious problem may arise because the complex amplitude of the signal wave may only be specified and controlled on a finite sampling grid. The corresponding physical wave field is determined by the interpolation of the sampled signal due to the finite size of the DE. Thus, the phase of the signal wave defined on the sampling grid clearly influences the intensity of the signal between the sample points. Due to the discrete definition of the signal strong intensity fluctuations may occur in the physical wave field. These fluctuations are normally referred to as speckles.

Figure 1 presents different forms of intensity fluctuations and their corresponding phase distributions. It shows the computer-simulated intensity of the physical signal wave generated by a DE (lower-left). The obvious intensity fluctuations of the generated signal wave can be divided into two types, fluctuations caused by spiral phase singularities (upper-right and upper-left) and fluctuations originating from neighbouring sample points with a phase difference close to π without forming a phase singularity (lower-right). The latter type consists of intensity fluctuations only close to zero. As stated in the next section, the first type is actually a zero location of the signal wave. This zero location lies on an optical vortex of the propagating EM field. We will refer to an intersection of an optical vortex with the observation plane as a speckle or phase singularity. It should be mentioned that in certain cases spiral phase singularities are needed in the design of DEs performing map transforms on the incoming wave [9, 10].

An approach based on an IFTA to avoid speckle problems in the design of diffractive amplitude elements (DAE) of the Fourier type has been proposed in [11, 12]. In this paper we present an extended design concept which can be used to determine transmission functions of DEs of the Fourier or Fresnel type fulfilling almost any restriction to the modulation domain without speckles in the physical signal wave. Because of their practical importance we focus our methods on the design of diffractive phase elements (DPE). These elements are characterized by perfect transparency and thus by optimal diffraction efficiencies. In section 2 the theory of speckles is consolidated to get a better understanding about the nature of speckles which turns out to be useful for the development of methods avoiding or removing speckles during a design process. In section 3 the influence of the signal phase on the DPE design is examined. A soft coding method avoiding speckles during the DPE computation is presented in section 4 and finally an algorithm to remove pairs of speckles is introduced in section 5.

2 Theory of Speckles

A point in the phase distribution of a wave front is called spiral phase singularity if all phase values between 0 and 2π can be found in an arbitrary small surrounding around the point. Such a point must be a zero location of the wave front. In the following a relation between the order of the zero location and a property called the order of the spiral phase singularity will be derived.

Let $f(x) = f_{\rm R}(x) + i f_{\rm I}(x)$ with $x = (x_1, x_2)$ be a complex-valued infinitely many times continuously differentiable function specifying a scalar wavefront in a certain plane. The integral

$$S(f, x_0) := \frac{1}{2\pi} \int_{\Gamma_{x_0}} (\nabla \arg f) (x) \cdot dx = \frac{1}{2\pi} \int_{\Gamma_{x_0}} \frac{f_{\rm R} \nabla f_{\rm I} - f_{\rm I} \nabla f_{\rm R}}{|f|^2} \cdot dx, \quad (1)$$

where Γ_{x_0} is a sufficiently small positively oriented simple closed curve around x_0 with $f(\Gamma_{x_0}(t)) \neq 0$, defines the order of the spiral singularity of the phase of f(x) in the point x_0 . We will show that $S(f, x_0)$ is an integer and that x_0 has to be an isolated zero location of f(x) if $S(f, x_0)$ is not equal to zero. We will call such a zero location a *speckle* of order $k = S(f, x_0) \in \mathbb{Z}$. If $S(f_1, x_0)$ and $S(f_2, x_0)$ is defined for two functions f_1 and f_2 it is obvious that

$$S(f_1 f_2, x_0) = S(f_1, x_0) + S(f_2, x_0)$$
 and (2)

$$S(a, x_0) = 0 \quad \text{with} \quad a \in \mathbb{C} \tag{3}$$

hold.

Because f(x) is infinitely many times continuously differentiable in the point x_0 , f(x) may be developed in a bivariate power series around x_0 . Without loss of generality we let x_0 coincide with the origin (otherwise consider $f(x - x_0)$) and get

$$f(x_1, x_2) = \sum_{m=0}^{\infty} \sum_{l=0}^{m} a_{ml} x_1^l x_2^{m-l}$$
(4)

with complex coefficients a_{ml} . The behaviour of f(x) in the vicinity of the origin may now be described by considering only the monomials of the least order n with non-zero coefficients, i.e. $S(f, x_0) = S(\hat{f}, x_0)$ with

$$\hat{f}(x_1, x_2) := \sum_{l=0}^{n} a_{nl} x_1^l x_2^{n-l}.$$
(5)

If n > 0, x_0 is a zero location of order n and \hat{f} may be factorized uniquely as

$$\hat{f}(x_1, x_2) = b_0 x_1^p x_2^q \prod_{m=1}^{n-p-q} (x_1 + b_m x_2)$$
(6)

with complex constants $b_m \neq 0$ and $p, q \in \mathbb{N}_0$. The point x = 0 is an isolated zero location of f(x) if and only if p, q = 0 and $\operatorname{Im}(b_m) \neq 0$ for all

 $m \in \{1, \ldots, n\}$. Otherwise f(x) contains zero lines through the point x = 0 as described in [13].

It can be shown that

$$S(x_1 + b_m x_2, 0) = \operatorname{sign}(\operatorname{Im}(b_m)) = \begin{cases} -1 & \text{for } \operatorname{Im}(b_m) < 0\\ 1 & \text{for } \operatorname{Im}(b_m) > 0, \end{cases}$$
(7)

holds whereas, as already mentioned, $\text{Im}(b_m) = 0$ does not occur in the case of isolated zero locations. With equation (2) we achieve

$$S(f,0) = \sum_{m=1}^{n} S(x_1 + b_m x_2, 0).$$
(8)

Thus, a zero location x_0 of order n is a speckle of order $k = S(f, x_0)$ with $|k| \leq n$. Figure 2 shows the amplitude and phase distribution of speckles with order k = 1, k = 2, k = 3 and k = -1, respectively. The three leftmost speckles are zero locations of order n = k, whereas the speckle to the right is a 3rd.-order zero with a spiral phase singularity of order $k = -1 \neq n$.

One should be aware of the fact that a spiral phase singularity of order k leads to zero location of order $n \ge |k|$. On the other hand, an isolated zero location of order n does not necessarily lead to a spiral phase singularity. This is only true whenever n is odd. If n is even, the sum in equation (8) could add up to zero.

As already stated in [14] speckles of order $|k| \ge 2$ are very rare. This is due to the fact that small perturbations of the wavefront tend to split a higher order zero location into several zero locations of order 1, thus limiting the absolute value of the order of the corresponding speckles to 1. Likewise, zero lines tend to be split into isolated zero locations according to Eisenstein's criterion [13].

Considering the lines of a constant phase φ of $\arg(f(x))$ it becomes clear that every speckle of order 1 is connected to exactly one speckle of order -1 and vice versa under the assumption that f(x) does not possess any zero locations of order n > 1. We refer to two corresponding speckles as a *speckle pair* (top-left of figure refrealspecs). These pairs are not unique, i.e. by choosing another φ other speckle pairs may be built. The lines of the constant phase φ never intersect, but may touch one another. This leads to the fact that there is always an equal number of speckles of order 1 (positive speckles) and -1 (negative speckles).

3 The influence of the signal phase

As mentioned above algorithms such as IFTAs, DBS or SA for the computation of DEs generating desired intensity signals only control the intensity in discrete points of the generated continuous wavefront. The phase of these sample points has an enormous influence on the intensity distribution between the points. If the phase difference of two neighbouring sample points is close to π , the intensity of the continuous distribution between these two points is likely to possess a minimum value close to zero. The way the sample points have to be interpolated in order to describe the optical output depends on the form of the finite sized element and whether the signal lies in the Fourier or Fresnel region of the DE.

One possibility to control the intensity between the sample points is simply to supersample the generated intensity signal and optimize the DE in terms of this supersampled signal. This method works well for all intensity fluctuations except for fluctuations caused by spiral phase singularities. These zero locations cannot be removed by local changes of the intensity of the generated wavefront. Standard optimization techniques are all based on local changes of the sample points, i.e. the sample points are independently optimized. One approach applying global changes was given in [15].

Because IFTA cannot remove zero locations in the signal wave caused by spiral phase singularity the initial signal phase distribution has to be carefully chosen. Two requirements should be fulfilled by the chosen signal phase. First, the phase distribution should not possess phase singularities because these would induce zero locations in the physical signal wave according to section 2. Secondly, the signal phase should distribute the entire signal energy as uniformly as possible into the region $W_{\rm DE}$ in which the DE is located when applying the inverse wave propagation operator. Such a signal phase is a well-chosen starting point for the iterative optimization process because the amplitude of the inverse wave propagation of the complex signal is close to the constant amplitude of a DPE. These requirements will in the following be examined for four different signal phases; a constant, random, pseudo-random and spherical phase $\varphi(x) = \exp(i\alpha |x|^2)$. The intensity distribution in figure 1 is used as an illustrative example of a signal wave in the general beam shaping problem. Of course any other intensity signal could be used.

We combine the amplitude of the signal in figure 1 with each of the above phase distributions leading to four different complex-valued signal waves. Figure 3 shows the inverse wave propagation of the signal waves. Obviously, the constant phase does not distribute the energy of the signal wave uniformly into the DE window. Thus, the amplitude distribution in the DE Window is very different from the constant amplitude of a DPE. The other phase distributions show a much better uniformity of the energy distribution in the DE window and are thus better suited as initial phase distributions in the design of a DPE. The initial phase may be further improved by a pre-iteration finding an object-dependent initial signal phase [12].

Because the constant signal phase distribution did not fulfil the second requirement we continue by using the signal waves with a random, pseudorandom and spherical phase for a DPE design for the general beam shaping problem. We will in the following compute DPEs using an IFTA with equal computation costs for all three signal phase distributions. Figure 4 shows the flow diagram of a general IFTA as described in [16]. The operators \mathcal{U} and \mathcal{X} are applied in every step of the iteration process in order to fulfil constraints on the DE and the signal, respectively. These are normally projections onto the desired subset, i.e. the set of "fabricatable" DEs and that of acceptable signals.

Without a significant loss of generality, we consider a DPE design assuming a plane illumination wave and a Fourier propagation operator. For the computation of a continuous DPE F(u) which is defined in a window W_{DE} and generates a desired intensity distribution $|s_0(x)|^2$ in a signal window W_{Signal} the operators \mathcal{X} and \mathcal{U} may be defined as

$$(\mathcal{X}s)(x) := \begin{cases} \alpha |s_0(x)| \exp(i \arg s(x)) & \text{for } x \in W_{\text{Signal}} \\ s(x) & \text{otherwise} \end{cases}$$
(9)

$$(\mathcal{U}_{\text{hard}}F)(u) := \begin{cases} \exp(i \arg F(u)) & \text{for } u \in W_{\text{DE}} \\ 0 & \text{otherwise} \end{cases}$$
(10)

with α being a free scale parameter as described in [16, 17].

The amplitude of the signal waves of the computed DPEs are shown in figure 5. The left image depicts the DPE and its signal wave in the case of the random initial signal phase. This phase distribution definitely contains spiral singularities. As can be seen from figure 5, these could not be removed by an IFTA. The middle image was computed with a special object-independent phase distribution designed by Bräuer et al. [12]. This is a non-deterministic phase distribution without spiral phase singularities but at the same time a good diffuser as shown in figure 3. The number of speckles could be significantly reduced. However, the hard projection operator \mathcal{U} tends to change the signal phase dramatically during the iteration process. This usually introduces spiral phase singularities which again leads to speckles. In the right image of figure 5 a spherical phase distribution was applied. The continuous spherical phase does of course not contain any spiral phase singularities. This also holds for the sampled version unless the sampling criterion is violated. The smoothness of the spherical wave seems to prevent the introduction of spiral phase singularities in the signal wave during the iteration process.

At first glance a suitably chosen spherical signal phase seems to be ideal for solving the general beam shaping problem. However, a spherical signal phase leads to often undesirable imaging properties of the DE. A consequence is the effect of perturbations of the DPE distribution due to damages, dust or a varying illumination wave. This effect is illustrated in figure 6 for a pseudo-random and a spherical signal phase. It can easily be seen that the DPE computed with the initial pseudo-random signal phase spreads the local error over the entire signal window, whereas the DPE with the initial spherical signal phase rather images the error into the signal window.

If the modulation constraints of the DPE are harder to fulfil than those of the above examples, e.g. if a quantized phase element is to be computed, speckles may occur even when the DPE was computed with an initial spherical signal phase. In this case, or if the imaging property of the spherical phase is unwanted, the above method can be improved by introducing a soft coding operator.

4 Soft coding

The hard projection \mathcal{U} tends to change the phase of the signal wave $\hat{s}_k = \mathcal{X} s_k$ dramatically from one iteration step to the next. Such a hard operator thus leads to a lack of control of the signal phase initiated by the carefully chosen initial phase and may cause spiral phase singularities in \hat{s}_k . In the case of a discrete intensity signal in which the phase is a complete parameter of freedom such changes are of no concern. However, when computing DPEs for continuous intensity distributions only a *restricted* phase freedom may be used in the optimization process, i.e. the phase distribution of the signal may develop freely as long as no spiral singularities occur during the iteration process. One possible way to achieve this is to choose an appropriate initial signal phase and apply a soft operator

$$\mathcal{U}_{\text{soft}} := \beta \, \mathcal{U}_{\text{hard}} + (1 - \beta) \, I \tag{11}$$

where β is a parameter of progression going from 0 to 1 during the iteration process and I the identity operator. $\mathcal{U}_{\text{soft}}$ leads to minimal changes in the phase of s_k , thus avoiding spiral phase singularities to arise. It is perfectly permissible to apply such a soft operator because F_k only has to fulfil the DPE constraint at the end of the iteration process and not after every iteration step. However, also soft operators cause changes in the phase distribution of \hat{s}_k . Thus, it is important that the initial phase distribution allows minor changes without introducing spiral phase singularities.

Figure 7 (left column) shows the generated signal wave of a DPE computed with an initial pseudo-random phase and the soft operator defined in equation (11). Other boundary conditions were the same as in the previous section. Compared to figure 5 the amplitude of the signal wave shows only a few speckles. However, it may happen that they cannot completely be removed by the iteration. Thus an additional method for removing the remaining speckles has to be developed.

5 Removing pairs of speckles

From section 2 we know that normally only speckles of order ± 1 occur in practice and that these build pairs of speckles. Hence, it is *impossible* to remove a single speckle no matter how the amplitude, phase or both of the phase singularity are smoothed because this violates the equality of positive and negative speckles. In the case of IFTA the removed speckle will definitely reappear in the next iteration step. The only way to overcome this problem is to remove pairs of speckles. Therefore we need a method to identify speckle pairs which will be derived from the following line integral.

Let B be a simply connected region in \mathbb{R}^2 . We will call

$$S(f,\partial B) := \frac{1}{2\pi} \int_{\partial B} (\nabla \arg f)(x) \cdot dx \tag{12}$$

where ∂B denotes a positively oriented simple closed curve around B the *speckle number* of f in region B. If the interior of B contains n isolated zeros x_1, \ldots, x_n of f, it can be shown that

$$S(f,\partial B) = \sum_{m=1}^{n} S(f, x_m)$$
(13)

holds. Thus, if x_1, \ldots, x_n are all first order zero locations of f, $S(f, \partial B)$ is simply the difference between positive and negative speckles of f in B.

The integral can be used to find a small region B containing speckles which can be removed. If B only contains two speckles building a pair, $S(f, \partial B)$ must be zero. Such a pair can be removed with the following procedure. First, the signal phase of region B has to be smoothed so that B contains no spiral phase singularities. This is always possible when $S(f, \partial B) = 0$. We applied a simple smoothing algorithm setting the phase of an inner point to the weighted sum of the phase values on ∂B with weights depending on the distance. Then a standard optimization algorithm—for instance an IFTA—should be applied with no freedom of phase in B so that the forced phase alteration can be evenly distributed over the entire signal distribution. One advantage of soft operators is to limit widely separated speckle pairs to a minimum which is very helpful for later removement of speckle pairs. A result of the above described procedure is shown in the right column of figure 7. If a small region contains several speckles the speckle cluster (larger circle) can be removed if the line integral is equal to zero.

6 Conclusion

We have stated the point that the phase distribution of intensity signals cannot be used as a complete parameter of freedom for the optimization process of DEs generating a signal wave specified on a continuous support in the Fresnel or Fourier region. A "restricted phase freedom" must however be used in order to achieve a high quality element.

A mathematical definition of speckles in wavefronts was given. Based on this definition a speckle of order k could be described as an n-fold isolated zero location of the wavefront with a spiral phase singularity of order k, where $|k| \leq n$ holds. This theory turned out to be useful for creating strategies for avoiding speckles during an iterative design process. Because IFTA is not capable of removing speckles caused by spiral phase singularities in the signal wave, the importance of using an initial signal phase without phase singularities was emphasized. Different signal phase distributions were examined and compared. An interesting result is that a spherical phase is a very good initial phase for the design of a DPE if imaging properties of the DPE are acceptable. The presented iterative design algorithm was used to compute continuous DPEs generating continuous signal waves without speckles if an initial spherical signal phase was applied. If an application does not allow the imaging properties introduced by a spherical phase an initial pseudo-random signal phase should be used.

A further improvement of the method was achieved by introducing a soft coding operator with which the signal phase can better be controlled during the iteration process so that spiral phase singularities of the signal wave are not likely to appear. However, if speckles do appear these can be removed by a proposed method based on a line integral which can be used to find regions containing pairs of speckles. These pairs could be removed by applying a post-iteration with a restricted freedom of phase.

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Figure 1: Simulated signal wave generated by a diffractive phase element and some examples of intensity fluctuations. Each collection contains the amplitude (upper row) and phase distribution (lower row) as greyscale images (left column) and 3D plots (right column).





Figure 3: The capability of different signal phase distributions (upper row) to distribute the signal energy uniformly into the DE Window W_{DE} . The phase distributions are (from left to right) a constant, random, pseudo-random and a spherical phase. The corresponding amplitude distributions of the inverse wave propagation is shown in the lower row.



Figure 4: The flow diagram of a general IFTA (\mathcal{P} : wave propation operator, I: illumination wave, F_k : DE distribution of step k, s_k : generated signal of step k).

Figure 5: Amplitude distribution of the continuous signal wave generated by DPEs computed with an initial random (left), pseudo-random (middle) and spherical (right) signal phase distribution with the same computational costs (120 iteration steps).

Figure 6: The effect of a perturbation of the transmission functions (upper row) of DPEs computed with an initial pseudo-random signal phase (left column) and a spherical signal phase (right column) on the generated signal wave (lower row).

Figure 7: The amplitude and the phase of the signal wave generated by the DPE computed with the initial pseudo-random signal phase and the soft operator $\mathcal{U}_{\text{soft}}$ (left column). In the right column the speckles in the circumscribed regions were removed by a method applying a restricted freedom of phase.