Investigation of the basic properties of phase singularities generated by a phase bar or trench

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Abstract

In the present paper, we determine the conditions necessary for the generation of phase singularities in the far-field by a phase bar or a trench. The ultimate goal of our work is to link object parameters to a topological distribution of pairs of singularities. We apply scalar theory and show that objects smaller than the diffraction limit are not capable of generating singularities. Supplementary rigorous electromagnetic theory is applied to determine this feature size for a real structure. Topological behavior by changing a typical object parameter and stability of the position of phase singularities in the presence of neighboring scatterers are analyzed.

Keywords: Phase singularities; High-resolution microscopy; Diffraction

1. Introduction

Phase singularities are points in space where the real and imaginary parts of an electromagnetic field are equal to zero, meaning the intensity is always zero and consequently the phase becomes undetermined. A description of their basic properties and a resulting classification were given by Nye and Berry in the mid 1970s [1]. Basically, one distinguishes between edge, screw and mixed dislocations. They appear in various optical schemes. A perspicuous example for an edge dislocation, a line along which a phase jump of \( \pi \) occurs is, e.g., a simple Gauss–Hermite laser mode with the mode parameter 01. That laser mode has an intensity equal to zero along a certain axis (e.g., \( y \)-axis) and the phase difference in the waist between the field in space with \( y > 0 \) and in \( y < 0 \) is equal to \( \pi \). The phase at \( y = 0 \) cannot be defined. Screw dislocations are a common feature in wave fields that contain speckles. Their randomly distributed points with zero intensity are intimately related to screw dislocations [2]. Phase variation on a closed circle around a screw dislocation is always an integer multiple \( n \) of \( 2\pi \), which offers the possibility

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of measuring the location of the phase dislocation quite precisely by means of interferometric techniques. Tyehinsky and co-workers [3,4] proposed in a pioneering work at the end of the 1980s the use of structural features within a phase-field to reconstruct unknown object properties with the ultimate target of overcoming the classical resolution limit. The classical resolution limit, as we will understand it, is the smallest distance between two scattering objects such that they can be resolved in the far-field. The two objects in the present work are the two edges of the phase structure and for the resolution limit in the course of time different criteria have been derived. One of the most commonly used criteria for optical systems is the two-point resolution limit. By using this criterion, the minimum resolvable distance between two points for an incoherent system reads as \( \Delta x = 0.61 \frac{\lambda}{NA} \), with NA being the numerical aperture of the system [5]. If the imaging system is aberration-free, the smallest resolvable distance for a given wavelength scales with the numerical aperture, which limits the diffracted spatial frequency transmitted by the system. If the optical system is aberration-free, it is also called diffraction limited. Nonetheless, the conclusions of Tyehinsky et al. about the potential to exceed that limit in lateral dimensions were somewhat contradictory and the answer to the question whether it is possible to reach superresolution using phase singularities is still open. They outlined the problem of necessary a priori knowledge about the structure, which permits the correct interpretation of measured phase distributions. Other fundamental problems in using phase information for object reconstruction are the non-trivial response of the object, especially if its feature sizes are comparable to the wavelength. Unfortunately, to the best of the authors’ knowledge, no inverse rigorous interaction calculation exists that would permit reconstruction of the object parameters from measured wave-fields and the overall availability of phase contrast. Phase contrast describes the introduced difference in the optical path between the scatterer and its surrounding. The best resolution in terms of phase contrast within the scalar approximation is obtained for \( \pi \)-phase shifting objects. Subsequent investigations by Totzeck and Krumbügel [6] lead to comparable results. Additionally, they applied rigorous diffraction theory in order to compare theory and experiment exactly. In a more recent publication [7], Eberler, Dorn and co-workers investigated the topological behavior of phase-singularities generated by high-permittivity scatterers in reflection. In their conclusion, they outlined likewise the necessity of applying rigorous interaction theory in order to enable inference of structural features from measurements. Phase singularities that appear in the transmitted region of a sub-wavelength slit in a silver film have been investigated by Schouten et al. [8]. In their work, the authors analyzed topological events like creation and annihilation by changing the size of the slit.

The present work addresses the derivation of necessary conditions for the appearance of phase singularities generated by a phase bar or phase trench and the topological behavior of these phase singularities after changing object as well as system parameters. We try to find an answer to whether it is possible to resolve objects with feature sizes below the classical diffraction limit (superresolution). We limit our investigation to topological information transported in the far-field, because features below the diffraction limit can be resolved by taking evanescent waves into account [9]. The paper is structured as follows.

In Section 2, the basic geometry of the structure under investigation is presented and the numerical tools used are outlined. In Section 3, we apply scalar theory to find analytically an inequality which determines the smallest width of a phase bar, introducing a given phase delay, that is capable of generating phase singularities in the far-field. It is shown that a cooperative scatterer (a scatterer which introduces a maximum phase shift of \( \pi \)) must have at least a width of approximately \( \lambda/4 \), in order to generate phase singularities in the far-field. In Section 4, we will investigate the interaction problem rigorously and derive a set of requirements on the object as well as on the system, in order to generate phase singularities in the far-field with a feature size of the scatterer being as small as possible. This feature size is determined.

In Section 5, the topological behavior of phase singularities is investigated, by changing a typical
object parameter, i.e., its width. In the last section, stability of the position of phase singularities in the presence of neighboring scatterers is discussed.

2. Description of the basic problem and its numerical treatment

Fig. 1 depicts an example of the basic setup under investigation. It shows the resulting intensity and phase (isophase) distribution upon interaction of a plane wave with a phase bar. For all the figures, the intensity is defined for TE polarization as $EE^\ast$ and for TM polarization as $HH^\ast$. To simulate realistic objects, the phase bar has been chosen in our investigation not as a free-standing object, but rather as a feature on the surface of a substrate (trench or real bar, we have assumed the typical refractive index for glass and some plastics of $n = 1.5$). The problem is treated only for two-dimensional objects. They are invariant in the third direction. The trench in the surface (height $h = 0.488$ μm, width $w = 0.3$ μm) is illuminated from air along the $z$-axis by a plane wave (TM polarization). Turbulences appear in the wave-field, introduced by the perturbation. Two small circles mark the two edge-type phase singularities, which are directly related to the perturbation. Comparison of intensity and phase distribution makes it evident that the dislocations are intimately associated with an intensity equal to zero. The entire field distribution is low-pass filtered, assuming a numerical aperture equal to unity. The field in the transmitted region ($z > h$) is therefore in principle accessible by a far-field lens system (such as a high-resolution interference microscope working in transmission [10,11]) and can be measured. In practical applications, the absolute position of phase singularities relative to the structure under investigation for measurements in the far-field is the subject of ambiguity, because identification of the reference plane with the desired accuracy is not possible in a simple set-up. Consequently, we will investigate the relative distance between dislocations. That procedure is supported by nature, because phase singularities generated by the analyzed structure appear in pairs. It has to be pointed out that edge dislocations can also be generated using holographic optical elements without appearing pairwise [12].

For the numerical simulation of the interaction problem, various techniques have been implemented and tested. Nonetheless, most of the calculations have been made using rigorous grating theories. Details about Rigorous Coupled Wave Analysis (RCWA) and the Fourier Modal Method (FMM) can be found in the literature [13,14]. They are omitted for reasons of brevity. These theories make use of periodic boundaries, meaning that the structure is considered to extend periodically (the virtual boundary) for an infinite distance outside the region to be calculated. In preliminary computer experiments, we have investigated the necessary conditions for the calculation of aperiodic objects. A critical parameter is the virtual period for the object used in the calculation. For the sake of clarity, a sketch of the two geometries under consideration is shown. Fig. 2 shows the geometry for calculating the field distribution for a pure single element and in Fig. 3 the geometry with periodic boundary conditions. To estimate the influence, least square differences defined as coupling coefficient

$$z = \frac{1}{w} \int_{-w/2}^{w/2} (u(x, h)_{RCWA} - u(x, h)_{MoM})^2 \, dx$$
between the field of a single element and the field calculated with periodic boundary conditions were specified directly behind the structure as a function of the period. \( u(x, h) \) is the \( E_x \) component of the field for TE polarization and \( H_y \) for TM polarization. The field of the single element (no periodicity) was calculated using the Moment Method [15]. In Fig. 4, the coupling coefficient for a dielectric bar \( (n = 1.5) \) is shown. It has a height of \( \lambda \) and a width of \( \lambda/6 \). The bar is illuminated with a plane wave. Fig. 5 shows results of the same calculation for a bar having a width of \( \lambda/2 \). For both figures, the lower the value of \( \chi \), the better the periodic simulation matches the single element simulation. It is evident from the calculation that two conditions have to be fulfilled in order to use grating theories for the calculation of single elements. Firstly, one has to choose a period larger than three times the wavelength. Only by using such a period, can near-field coupling among different scatterers be neglected. By violating this condition, the coupling leads to intense and rapid alterations of the wave field as compared with the single element theory. Secondly, one has to choose a period in the calculation that is not an integer multiple of the wavelength. That period is critical because a diffraction order will propagate parallel to the grating vector and the resulting field suffers from multiple reflections from neighboring virtual objects [16].
3. Scalar prediction of smallest feature size capable of generating phase singularities

In this section, we will derive analytically the scalar prediction of the smallest width of a phase bar capable of generating phase singularities in the far-field as a function of its phase delay. The derivation starts for simplicity at the necessary condition for a grating to generate phase singularities. The field of such an object consists of a discrete number of plane waves. As mentioned in Section 1, a phase singularity appears if the field amplitude is equal to zero. This is only possible if the highest amplitude $a_n$ of the diffraction order $n$ is smaller or equal to the sum of all the other amplitudes $a_m$. This condition reads as [17]

$$\sum_{m=0}^{n-1} |a_m| \geq |a_n| \quad \forall n. \quad (1)$$

The highest amplitude in our setup $a_n$, is always the zero-order. In the absence of any structure, the zero-order is of course the only amplitude with a value different from zero. Introducing a perturbation will couple light into other diffraction orders and the strength of the zero-order will decrease. But it remains the order with the highest amplitude. Once the coupling into other amplitudes suffices to equal the zero-order, condition (1) is fulfilled and a singularity appears. Consequently $a_n$ is always $a_0$.

To extend the approach to single objects, we calculate the limit of Eq. (1) if the period tends to infinity. The summation becomes an integration and reads as

$$\int_{v} |a(v)|(1 - \delta(v - v_0)) \, dv$$

$$\geq \int_{v} |a(v)| \delta(v - v_0) \, dv \quad A \rightarrow \infty. \quad (2)$$

We will apply the thin element approach for the calculation of the amplitudes of the spatial frequencies. The basic idea of the thin element approach is that the transmitted field is given by a simple multiplication of the incoming wave-field and the transfer function of the structure, thus $F_{\text{trans}}(x) = T(x)F_{\text{inc}}(x)$ The transfer function of the phase bar is

$$T(x) = \begin{cases} 
 e^{i(2\pi h)/(n+a)}, & |x| \leq \frac{h}{2}, \\
 1, & |x| > \frac{h}{2},
\end{cases} \quad (3)$$

with $h$ the geometrical height. To calculate the far-field response of the structure the amplitudes of evanescent waves are excluded in the summation [18]. By using the thin element approach and Eq. (2), we derive a condition that determines the smallest width $w$ of a phase bar for a given phase delay $\Delta \phi$, in order to generate a phase singularity. It reads as

$$0 = 1 - \frac{4}{\pi} \sin \left( \frac{\Delta \phi}{2} \right) \int_{0}^{\infty} \left| \frac{\sin \left( \frac{t}{\lambda} \right)}{t} \right| \, dt. \quad (4)$$

Numerical evaluation for the right-hand side of Eq. 4 for three different values of an introduced phase delay $\Delta \phi$ are shown in Fig. 6. One can deduce from Fig. 6 that the smallest feature size for a cooperative scatterer $\Delta \phi = \pi$ capable of generating phase singularities in the far-field is $\approx \lambda/4$. This is comparable to the diffraction limit. If the introduced phase delay is smaller, a larger width is needed to have a phase singularity in the transmitted field. For further clarification of our analysis, the smallest amplitude in the transmitted field has been calculated for a $\pi$-scatterer as a function of its width. The value is shown in Fig. 7 together with the result of Eq. (4). It can be seen that the width where the field becomes zero coincides with the fulfillment of the condition for the appearance

![Fig. 6. Determination of the smallest width of phase bar which generates phase singularities in the far-field for three different phase delays.](image)
of singularities. Phase singularities are, as mentioned in Section 1, intimately related to a zero amplitude.

In conclusion from the analysis via scalar theory, we have to state that the promise of superresolution using phase singularities as information carriers at least with a single phase bar cannot hold up. They are only generated if the scatterer has a minimum width which is comparable to the diffraction limit. Smaller structures are not capable of doing so.

To treat the problem exactly, we apply in the following section rigorous electromagnetic theory and determine a set of parameters which are beneficial for generating singularities in the far-field with the smallest possible feature size.

4. Rigorous calculation of singularity appearance

4.1. Selection of polarization to illuminate a trench

The main question concerns the sensitivity to different kinds of structures using a wave of either TE (E-field oscillates along the space invariant y-direction) or TM (H-field oscillates along the space invariant y-direction) polarization as the illuminating beam. Sensitivity is for our purpose the possibility that a given object-system configuration can introduce turbulences in the phase distribution of a wave field, which leads to measurable phase singularities in the far-field. Two structures are distinguished. A positive one (trench) and a negative one (bar). Intensity and phase of the field distribution around a trench \( w = 0.2 \mu m, h = 0.488 \mu m, n_1 = 1, n_2 = 1.5, \Delta \phi = \pi \) illuminated with a TE-polarized plane wave are shown in Fig. 8(a) and for TM polarization in Fig. 8(b). Intensity for TE polarization is always defined as \( I = EE^* \) and for TM polarization as \( I = HH^* \). Field distributions are low pass filtered assuming again a numerical aperture of one. The wavelength is \( \lambda = 0.488 \mu m \). Black is equal to an intensity of zero, white is the maximum, which differs from figure to figure. Comparing the phase distributions after the trench shows that the TM polarization generates singularities, but in TE polarization the transmitted wave field remains plane. No pronounced turbulences appear for TE polarization. Note that the width of the trench in this example is larger than \( \lambda/4 \).

Explanation for this difference in the response is normally given by using waveguide theory [19]. A trench illuminated with a plane wave can be regarded as a resonator or as a small waveguide consisting of air, which acts differently for TE and TM polarization. If the surrounding material would be a perfect conductor, a TE mode would not be able to propagate within the trench if its width is smaller than \( \lambda/2 \) (cut-off wavelength). For the TM mode, no cut-off wavelength exists, the fundamental mode is always confined. A similar argumentation is true for high index dielectric materials and can be qualitatively applied to the present case. A TM mode excited within the structure receives a certain phase difference upon propagation relative to the field that propagates outside the structure. Interference leads to turbulences and hence to the generation of dislocations. A TE mode is not confined within the trench and hence no significant phase delays are introduced, the phase distribution remains plane. As a consequence, it is preferable to use TM-polarized light to create phase singularities in the far-field generated by a narrow trench.

4.2. Selection of polarization to illuminate a bar

Figs. 8(c) and 1(d) show the resulting field distribution from a bar of width \( w = 0.2 \mu m \) and
height $h = 0.488 \mu m$, $\Delta \phi = \pi$ with a plane TE-polarized (Fig. 8(c)) and TM-polarized (Fig. 8(d)) wave ($\lambda = 0.488 \mu m$) from air to glass. Phase singularities appear if the structure is illuminated with a TE-polarized wave, while for TM polarization the transmitted wave field remains plane and no singularity can be seen. This behavior is opposite to that observed for a trench (Figs. 8(a) and (b)). The explanation is likewise given by using arguments from waveguide theory. In the case of a high permittivity waveguide surrounded by air, a mode is always excited for both polarizations. The difference between the two polarizations is the propagation constant within the structure. The propagation constant is a function of the width and always higher for TE than for TM polarization. Consequently, the excited mode in TE polarization can accumulate a sufficient phase delay faster in order to interfere destructively with the transmitted plane wave in the outer region for smaller widths. Hence phase singularities are generated earlier in terms of feature size for TE polarization in the case of a bar.

An additional remark about the usefulness of detecting phase singularities, rather than measuring just intensity distributions in the far-field, can be made by comparing intensity and phase in Fig. 8. The intensity is smeared out over a relatively large area and small variations of object parameters would result in a small change of the intensity distribution, most likely inadequate to determine the variation of the width. On the other hand, the position of a phase singularity as an exact point in the wave field that can be measured
with high precision [11] and a small alteration of the objects leads to remarkable changes in the position of dislocations. This question will be discussed in the following section.

5. Smallest feature size that generates phase singularities

We have carefully evaluated the position of phase singularities, which can be directly related to the object under investigation as a function of its characteristic feature size. The case we are mainly investigating is the single trench illuminated with a TM wave. Calculations of absolute values, like distance of the dislocation relative to the structure (taking, e.g., \( z = 0 \) as reference) are not useful, because measurements in the far-field make it impossible to establish the reference plane precisely. Instead, we have used the fact that dislocations appear in pairs with opposite sign and their relative distance in the \( x \)-direction is a sufficient criteria, which can also be measured in the far-field without ambiguities. Because their appearance is symmetric, the \( x \)-distance between the center of the structure and the dislocation has been calculated. Fig. 9 shows the variation as a function of the width of a trench, illuminated with a plane TM-polarized wave. The fields have been low passed filtered using a numerical aperture of unity. The geometrical depth of the structure corresponds to one wavelength, which gives a \( \pi \)-phase shift for \( n = 1.5 \). Within the scalar approximation this would introduce the strongest phase turbulences. The arrow indicates the birth of the singularities. Values before that point are just distances between the points with highest phase gradient. It can be deduced from the figure that two points in the wave field exist with a highest phase contrast. If the structural feature reaches a value where the scatterer is capable of generating phase singularities in the far-field, these two points converge geometrically to the same position and the birth of a pair of dislocations takes place. The first phase singularity pair appears for the trench at a width of 0.17 \( \mu \)m. This width is larger than \( \lambda/4 = 0.488 \mu \text{m}/4 = 0.12 \mu \text{m} \). With increasing width, the distance between the dislocations increases quite linearly. It would be possible to deduce the characteristic object parameter by measuring the distance between the dislocations and using a priori knowledge about the structure. Such supplementary information on the structures are, e.g., the index of refraction of the material or the height of the object, because they have a significant influence on the distance between the dislocations. This information can be obtained from separate measurements or is known from the fabrication process and will hence simplify the precise determination of the unknown parameter. Additionally, it is in principle possible that different basic geometrical structures might generate the same pair of dislocations. To decide which geometry is the correct one, we have to know something about the geometry to exclude the implausible objects.

We deduce as the smallest feature size capable of generating phase singularities an object with a characteristic width of larger than \( \lambda/4 \), the predicted value of the scalar theory. This is due to the fact that the induced phase delay is not exactly \( \pi \) and the entire field distribution is smeared out while passing through the structure [20]. Smaller objects will not give strong gradients in the phase field.

Similar investigations have been made for a phase bar illuminated with a TE-polarized plane wave. All the other parameters remain constant. The behavior is different, as can be seen from
Fig. 10. Intensity and phase after illuminating a bar ($w = 0.16 \mu m$ in (a) and $w = 0.3 \mu m$ in (b), $h = 0.488 \mu m$) with a TE plane wave ($\lambda = 0.488 \mu m$).

Fig. 10(a) where a field distribution shortly after the birth of the singularity is shown. The width of the bar is $w = 0.16 \mu m$. Surprisingly, we found the same value for the smallest feature size capable of generating phase singularities in the far-field. But there is not a single pair but two pairs as for trenches. One can be found left of the structure, the other on the right. Fig. 10(b) shows the topological alteration of the wave field if the width is changed to $w = 0.3 \mu m$. The $x$-position of the singularities will change only negligibly. The main alteration takes place in the $z$-position. For completeness, Fig. 11 shows the $z$-distance between the two singularities as a function of the width of the bar. A TE-polarized plane wave was assumed for the illumination. In a way comparable to Fig. 9, it can be seen again that shortly after the birth the distance between the two singularities grows rapidly and will increase for somewhat larger phase bars to a good approximation linearly with the width. Measurement of these $z$-distances with high resolution is more time consuming, because a large space has to be scanned, but it is in principle possible [11].

It has to be stressed that all the values found are correct only for a refractive index equal to 1.5. If stronger scatterers are used, the nonlinearities appearing in the interaction are more pronounced and objects with a geometrical feature size smaller than $\lambda/4$ can generate phase singularities [21]. For optical systems having a numerical aperture smaller than unity, the lateral feature size for which a singularity appears in the diffracted field will be larger, but the subsequent linear relation between the width of the structure and the distance between the pair of singularities will remain [10].

To establish a relation between the distance of dislocations and unknown object parameters a second problem has to be investigated. This problem is the influence on the local position of the singularity if the system consists of more than one defect that serves as a scatterer in the closer surroundings. Simulation and discussions about the local stability of a phase singularity as a function of neighboring scatterers will be treated in the following section.

Fig. 11. Variation of the $z$-distance for phase singularities generated by a bar as a function of the width, TE polarization.
6. Stability of phase singularities in the presence of additional structures

First of all, in order to reduce the influence of scatterers in the closer surroundings, a Gaussian-distributed TE-polarized beam ($\sigma = 0.488 \mu m = \lambda$, waist at $z = 0$) has been used for illumination. We restrict ourselves to diffraction at a trench with neighboring trenches. The principal conclusions hold likewise for bars. TE polarization was used in the calculation because we can take advantage of faster computational procedure. A slightly larger width of the trench than the one necessary for the appearance of dislocations has been chosen. In Fig. 12, the change in the $x$-distance between the relevant phase singularities as a function of the distance $d$ between the central and the two neighboring trenches is shown (the geometry is shown explicitly in the inset of Fig. 12). The width of the trenches is 0.35 $\mu m$, the height of the structure is 0.488 $\mu m$ and the direction of the illumination goes from air ($n_1 = 1$) to glass ($n_2 = 1.5$). Ambiguous calculation, as indicated in the figure, means that the dislocation vanished either completely or its position can be just located outside the computational window. In both cases, identification of gradients in the phase distribution relative to the structure turns out to be cumbersome. We see that as long as the distance between the trenches is larger than the waist of the laser their position remains fairly stable. If the trenches are too close, coupling effects have a major impact on the resulting phase distribution and the position of the dislocation can no longer be linked in a simple manner to the structural feature. A re-calculation with increased resolution for distances far from the coupling region is shown in Fig. 13. From that and similar calculation, we have found that the distance $\Delta x$ between the perturbed dislocations oscillates more or less sinusoidally around the distance one would see for the unperturbed case. With increased distance the amplitude of the oscillation will be reduced. This behavior is attributed to components of the wave field that are reflected back and forth by the structures. Alteration of the distance between the trenches will change the optical path. Resulting variations between constructive and destructive interference of the diffracted wave will lead to the observed sinusoidal changes in the distance between dislocations.

If the optical system has a numerical aperture smaller than unity, the distance between the singularities for a given geometrical configuration is smaller. The influence of neighboring scatterers will be likewise negligible as long as the distance is larger than the waist of the laser. An excessive decrease will lead to the annihilation of the singularities. In each case, one has to compare the measurements with a calculation, assuming the specific set-up that was used in the experiment.

![Fig. 12. Variation of the distance $\Delta x$ between two dislocations generated by a trench of width $w = 0.35 \mu m$ as a function of the separation $d$ for two additional equal trenches.](image1)

![Fig. 13. Magnified distance variation from the example of Fig. 12 for a separation larger than a micron.](image2)
7. Summary

In the present work, we have derived conditions for the appearance of phase singularities as a function of object and system parameters for a phase bar and trench in transmission. By applying scalar theory to the problem, we have shown that the smallest width of a scatterer capable of generating singularities is somewhat wider than $\lambda/4$. This is comparable to the diffraction limit. We have applied rigorous electromagnetic theory to demonstrate the difference between a phase bar and a trench, both having the same phase delay. Likewise, we have shown that the smallest feature size capable of generating phase singularities in a rigorous calculation is comparable to the classical resolution limit, but larger than the predicted scalar value. If the structures are too small, no turbulences in the phase distribution can be generated. To have a singularity in the field, a point with zero intensity is required. Only relatively strong scatterers are capable of doing so. The explanation of the overall behavior has been given using arguments from waveguide theory. Nonetheless, once phase singularities appear, they will change their position quite rapidly by changing an object parameter. For the bar, the change in position is mainly in the $z$-direction, for the trench mainly in the $x$-direction. Illuminating the object under investigation with a focused Gaussian beam suppresses the influence on the position of generated phase singularities by neighboring objects. Only a resulting slightly sinusoidal variation of the position by changing the distance between neighboring scatterers remains. This is attributed to waves which are reflected back and forth by the structures.

Acknowledgements

The research was supported by the European Union within the framework of the Future and Emerging Technologies-SLAM program under Grant No. IST-2000-26479.

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