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Near-field focusing of an optical wave by diffraction gratings

Yu.E. Geints, A.A. Zemlyanov

Abstract. **We report the investigation results for spatially-localised light structures (photonic nanojets) under near-field optical radiation scattering on phase diffraction gratings. Main parameters of photonic nanojets from gratings with sawtooth, rectangular and hemispherical groove profiles are obtained by numerical electrodynamic simulation. It is found that by varying a period, degree of filling, groove shape and parameters of optically contrast coating of the diffraction grating one can control the characteristics of the produced photonic jets in a wide range.**

Keywords: *near-field focusing, diffraction grating, numerical electrodynamic simulation.*

1. Introduction

Modern optical technologies pertaining to material nanostructuring, precision diagnostics of parameters of dispersion media and ultra-sensing [1–3] require high spatial localisation of the electromagnetic field near objects under investigation, which often have nano-scale dimensions. As a rule, ultrahigh field focusing is realised by exciting so-called plasmon–polariton resonances near a surface of metal nanoparticles [4] or by employing field localisation on nano-tips [5].

In the last decade, the problem of such super-focusing in scattering of a light wave on transparent dielectric micro-objects having various geometrical shapes, structural composition and dimensions on the order of a wavelength of incident radiation (meso-scale particles) has been actively discussed in the literature [6–12]. Meanwhile a highly spatially localised intensive light flux is formed in a particle shadow, which was termed a 'photonic nanojet' (PNJ) [7]. Nature of the PNJ origin is related to the near-field aberration focusing of radiation by a transparent particle [13]. In this case, in the rear hemisphere, a lengthy focal domain is formed with an ultrahigh spatial resolution (up to sub-diffraction) and high intensity due to constructive interference of the light fields of radiation scattered and passed through a particle. The PNJ parameters can be efficiently controlled by varying the size, optical properties and shape of microparticles [6].

In practice, the employment of isolated microparticles for obtaining a PNJ is not simple because of the technical difficulties related to fixing a micron-size object in space. This is why presently the most popular method for obtaining and using a PNJ is placement of a great number of microparticles, for example, transparent hemispheres, on a surface of the irradiated sample [14–18]. In this case, particles on the surface are self-organised into single- or multilayer lengthy clusters. A substantial drawback of this technology is that the close packing of particles yields a strictly definite mutual disposition of the formed photonic jets and limits the possibilities of controlling their parameters.

From the viewpoint of physical optics, an ordered array of transparent microparticles is a phase plate with a periodically varying refractive index. A striking example of such media is a phase diffraction grating (DG) widely used in spectroscopy, image formation systems, etc. [19]. In contrast to conventional amplitude DGs, which usually operate in reflection, phase gratings are transparent for optical radiation and actually possess negligible losses of light energy. With a variety of construction types of DGs the main purpose of these optical elements is angular selection of spectral components in an optical signal and their concentration in certain spatial zones – zones of diffraction intensity maxima of the DG. Transverse dimensions of these maxima depend on the angle of observation and the size of a working range of the DG; the spatial localisation itself is determined by the grating period.

As a rule, DGs are used in the outgoing light, which is a far-field zone of electromagnetic wave diffraction on an obstacle. However, the optical field near the grating surface is also characterised by a strong spatial inhomogeneity, which is caused by interference of outgoing and surface (damped) waves [20]. The latter have a wavevector with a zero real part, cannot propagate to large distances, and damp at a distance on the order of the scale of the optical inhomogeneity of the diffraction element, that is, the DG period. By physical essence, the near-field diffraction of a light wave on a part of the DG relief is similar to forming a PNJ on a meso-scale particle possessing the same spatial shape and optical properties. In this case, the entire grating can be presented as an ordered array of such particles placed on a transparent substrate which generate localised light fluxes.

In the present work we, to our knowledge, consider for the first time the diffraction of an optical wave on a phase DG from the viewpoint of generating a PNJ ensemble near its surface. Based on numerical simulation of differential Maxwell equations we investigate the spatial and amplitude characteristics of arising photon fluxes under varying parameters of the diffraction gratings. It appears that the photonic jets from the DG, in contrast to microparticle self-assemblies, can be controlled by changing the shape of grating grooves, varying the spatial period of the grating, and depositing an antireflection coating.

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2. Results of numerical simulation

Three most popular types of phase gratings with grooves of triangular, rectangular and hemispherical profiles have been considered (Fig. 1). The triangular-groove diffraction grating (TDG) sometimes called an echelette or Wood grating, can efficiently concentrate light reflected from it in the range of spatial angles that is determined by the blaze angle of the grating, α. Such a grating with $\alpha = 30°$ is shown in Fig. 1a.

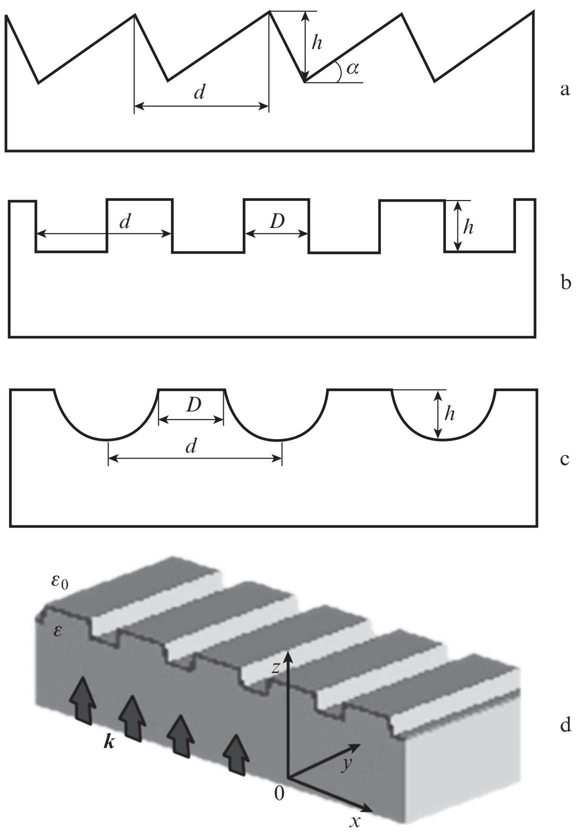

Figure 1. Transverse profiles of modelled DGs with (a) triangular, (b) rectangular and (c) hemispherical grooves; (d) scheme of optical wave (with a wave vector $\boldsymbol{k}$) diffraction on the DG.

Rectangular-groove diffraction gratings (RDGs), as a rule, are used for matching optical routes and switching optical signals between elements of photonic systems (Fig. 1b). Finally, hemisphere-groove DGs (HDGs) as in Fig. 1c are gratings for general purposes. All gratings are characterised by the period d and groove height h; RDGs and HDGs have an additional parameter, i.e. the filling factor $\kappa = D/d$.

Numerical calculation of the near-field structure in the case of light wave diffraction on a DG was performed by using our software package comprising the kernel C^{++} module of three-dimensional FDTD with an open source code [10], which was modified for particular calculation configurations. The software has been verified on test problems that have known analytical solutions: for example, the diffraction of a plane wave on a rectangular slit or scattering on a transparent sphere (Mie scattering). A three-dimensional configuration of the calculation domain was considered; inside this domain, according to a particular type of the DG, the profile of the dielectric constant ε in the coordinate axes $x - z$ was specified. It was assumed that the gratings are in air ($\varepsilon_0 = 1$) and are made of optical glass ($\varepsilon = 2.22$) with a zero dispersion in the optical wavelength range. The geometrical dimensions of the calculation domain were 7×7 μm at a total number of nodes $\sim 10^6$.

At the initial instant, on the bottom boundary of the calculation domain, a source of monochromatic radiation with a wavelength of $\lambda = 0.532$ μm was switched on. The source was presented as a plane linearly polarised wave with the electric field vector directed along grating grooves (y axis). The optical wave propagated through the DG in the positive direction of the z axis (Fig. 1d) and formed a near-field diffraction pattern of scattering, which was averaged over 1 ps. The spatial distributions of the relative field intensity $B(x,z) = |\boldsymbol{E}(x,z)|^2/E_0^2$ (E_0 is the incident wave amplitude) obtained in this way were analysed in order to find localised domains of elevated intensity, i.e., PNJs, and determine their dimensional and amplitude characteristics. For definiteness, in calculations we limited ourselves to a constant value of the groove depth in all DG types: $h = \lambda$.

Consider the structure of a PNJ in more detail from the viewpoint of influence of the type of a generative DG. We introduce the dimensional parameters of the photonic jet, which characterise it as a localised light structure, namely, the length L, width R and distance f from the grating surface (focal distance). The amplitude characteristic of the PNJ is a value of the peak (relative) optical field intensity B_m in the near-field scattering zone. The physical sense of these values is illustrated in Fig. 2, where the intensity profiles B are plotted near the TDG with $d = 2\lambda$, $\alpha = 45°$. Thus, the focal distance f describes a central position of the PNJ domain where the intensity of the light flux is maximal.

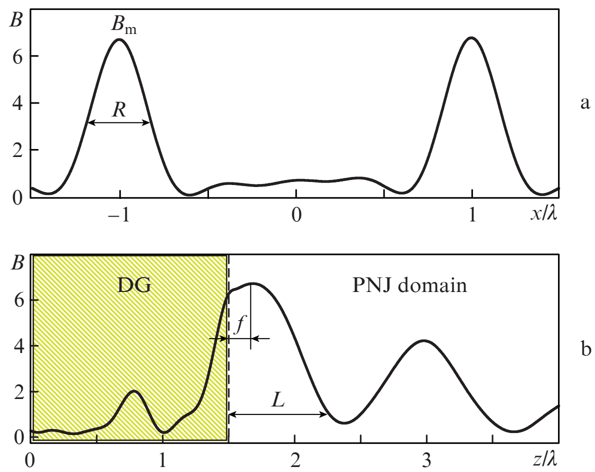

Figure 2. (a) Transverse and (b) longitudinal intensity profiles of a PNJ from the TDG. Vertical dashed line shows a DG boundary; the radiation passes from the left.

To avoid ambiguous meanings of PNJ parameters, in what follows we will define the width R at half the maximal field intensity level (FWHM), and the length of the jet L – at the fixed intensity level $B = 1$. For the integrated estimate of the degree of spatial localisation for the PNJ as a whole we will use the quality criterion Q [10], which comprises three main parameters of a jet: $Q = B_\mathrm{m} L/R$.

2.1. Triangular-groove gratings

We start our consideration with a PNJ formed by an echelette, i.e., a triangular-groove diffraction grating. As mentioned above, in addition to the grating period d, which will be assumed constant, the main characteristic of a TDG is the blaze angle α, which determines the far-field angular direction of the maximal concentration of energy passed through the phase grating.

A spatial distribution of the relative intensity B of the light field near the TDG is shown in Fig. 3a for the incident wavelength λ =0.532 μm. One can see that in this case a spatially localised optical structure is formed. Following the tradition we will call this structure a photonic nanojet. The spatial shape of the PNJ is sufficiently complicated and comprises a system of maxima and side lobes. The intensity and dimensional parameters of this PNJ vary with the blaze angle (Figs 3b and 3c) and depend on the DG type.

In the near-field scattering zone, a variation of the blaze angle, as follows from the figure, mostly affects the length, intensity and focal distance of the formed PNJ and relatively weakly changes its width. The PNJ itself, regardless of the value of α, has no inclination and is always directed along the wave vector of the incident radiation. For two extreme values of the DG blaze angle, the quality parameters of the jet differ actually twice, reaching a maximum Q = 40 for the grating with grooves in the form of an isosceles triangle (α = 45°). In this case, the thinnest photonic jet is realised with R = 0.37λ and $L \sim 2\lambda$. At the same time, in the case of mostly asymmetric shape of grating grooves (α = 15°), the jet length sharply increases; however, its spatial localisation worsens. All PNJs from a triangular profile grating are formed sufficiently close to the output face at an average focal distance f equal to λ/2.

The fact of optical field localisation and PNJ origin in diffraction of a light wave on a DG is related with the transverse optical phase gradients, which are produced by grooves, i.e., spatial inhomogeneities on the surface of the grating. Obviously, the sharper the phase gradient, the higher the optical field localisation. In a triangular-groove DG, the phase increment of the optical wave passing through a groove changes linearly; this results in the so called conical type of field focusing.

Analysis of the temporal dynamics of the PNJ formation in the case of a TDG shows that blurring of spatial boundaries of a light flux in gratings with a small blaze angle is related to the fall of the optical phase gradient due to a greater length of one of the groove faces at the expense of the other. The longer, hence, at a constant period, more gently inclined face of the groove results in a softer conical focusing of the wave by the groove. Finally, this yields a more distant from the grating, wider, and lengthy focal spot.

2.2. Rectangular-groove gratings

Diffraction gratings with fixed groove profiles are interesting for generating localised light fluxes because in such structures the PNJ parameters can be easily controlled by direct variation of the groove width (the filling factor) within the limits of the grating period. Indeed, if we still consider inhomogeneities on the grating surface as focusing elements with the converging action dependent on their spatial profile then, for example, an increase in the groove width will be similar to an increase in the geometrical aperture of elementary lenses and their optical efficiency. At the same time, the local curvature of the phase wavefront at the output from grooves will reduce, which will result in a longer equivalent focal length of such lenses and a reduced optical efficiency. As a result, in approaching a balance between these tendencies, an optimal configuration of the groove can be found which forms a PNJ of the highest quality.

Let us analyse Fig. 4, where the main parameters of the PNJ formed by RDGs with various filling factors are presented. As previously, the groove depth h and grating period d are constant and equal to λ and 2λ, respectively.

Indeed, in contrast to the case with a triangular groove profile (Fig. 3a), Fig. 4a shows that a sufficiently noticeable extremum in the PNJ quality criterion is observed near the filling factor value $\kappa \approx$ 0.27. The maximum of Q itself is more

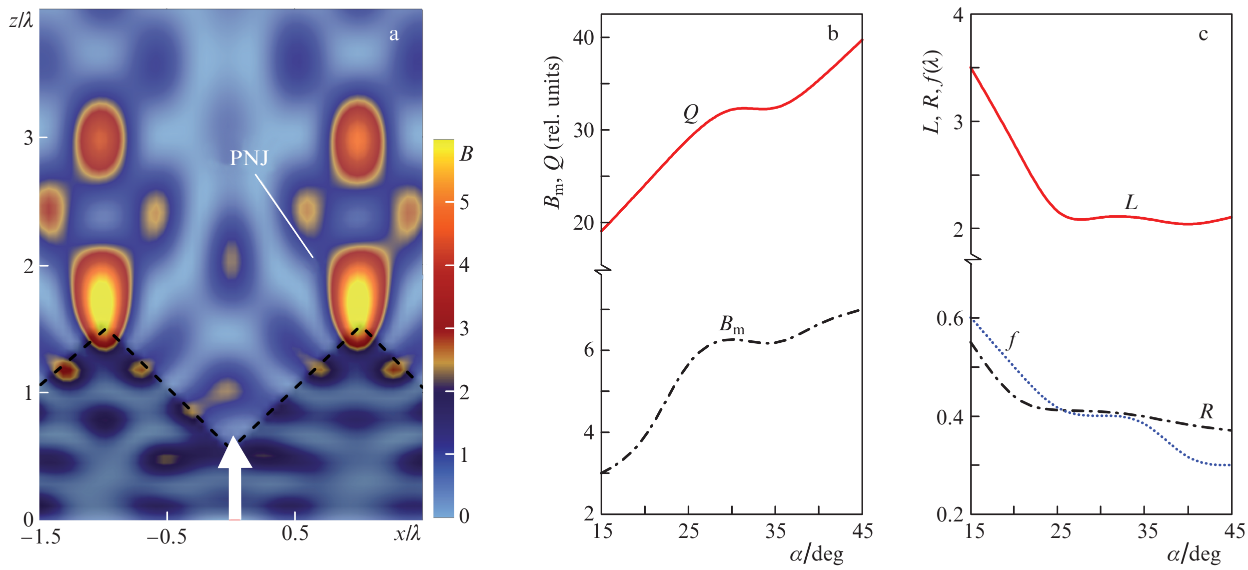

Figure 3. (Colour online) (a) Spatial profile of the intensity B of an optical field near the TDG and (b, c) main parameters of the PNJ vs. the blaze angle α. Arrow shows the direction of radiation incidence.

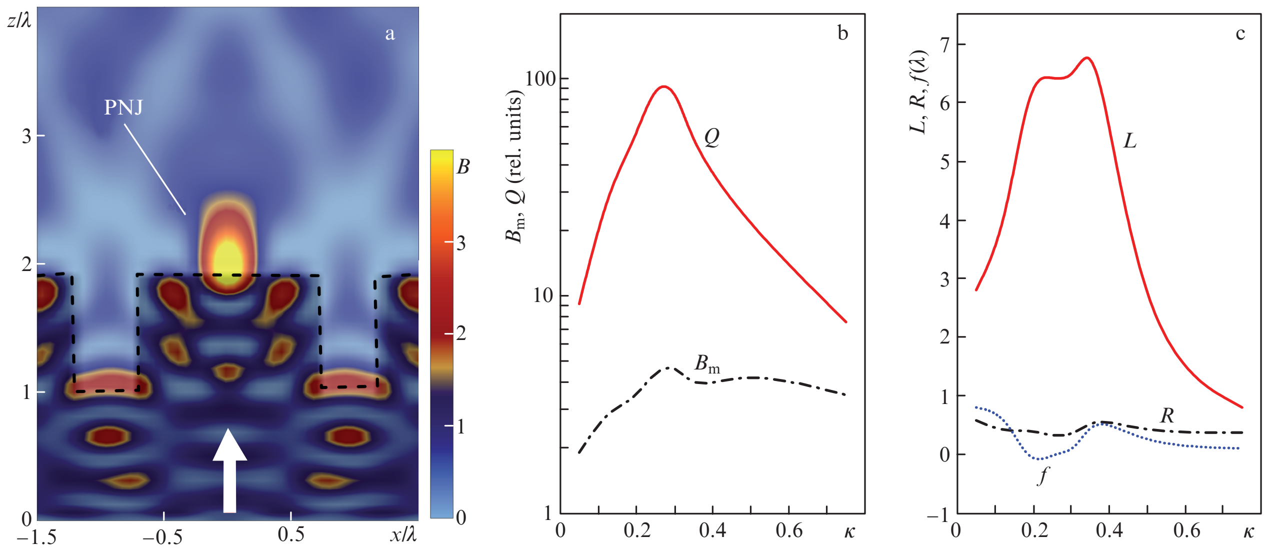

Figure 4. (Colour online) Same as in Fig. 3, for a RDG at a varying filling factor.

than twice greater than a similar peak value in the case of the TDG. If we turn to Fig. 4b, then it becomes clear that this enhancement of the photonic jet quality is related both to its higher localisation in the transversal direction, and to the noticeable elongation of the PNJ. The minimal possible width of the PNJ obtained from calculations in the case of a RDG is $R = 0.3\lambda$ at the maximal realised length $L \approx 7\lambda$. For the TDG these parameters are worse: $R = 0.34\lambda$ and $L = 3.5\lambda$.

In gratings with a wider separation between grooves ($\kappa <$ 0.2) part of energy 'intercepted' by grooves reduces, which leads to a fall in the peak intensity in the focusing domain and worsens jet parameters. At a higher filling factor, the mutual overlapping of the fields of spatial modes emitted by neighbouring grooves becomes substantial and leads to numerous interference fringes; this breaks photonic jet localisation and deteriorates its quality.

One more feature of RDGs is that PNJs with a high quality factor are formed actually near groove edges. As follows from Fig. 4b, at $\kappa = 0.2-0.35$ the jet focal distance f is almost zero, which testifies that the jet adjoins the DG. Moreover, at $\kappa = 0.2$ the maximum of the optical field intensity is inside the grating groove, and the photonic jet 'escapes' through its surface with an exponentially falling intensity. This fact is taken into account in the form of a negative value of the focal distance of such a jet ($f = -0.2\lambda$).

2.3. Hemisphere-groove gratings

Diffraction gratings with hemispherical groove profiles exhibit features of both types of the DGs discussed above. Indeed, the side faces of grooves generating photonic jets in such a grating are sufficiently gentle, which should provide focusing of passing radiation into a spot with compact dimensions similarly to a RDG. On the other hand, in HDGs the end face of grooves is, as a rule, plane and, similarly to a RDG, serves as an emitting waveguide aperture. Hence, we may expect formation of a lengthy focal domain in this type of the DG.

The main characteristics of the PNJ produced by a HDG are presented in Fig. 5. In numerical simulation, the profile of grating groove remained constant and was a hemisphere with a radius equal to the wavelength (for definiteness); the varied parameter was the distance D between grooves (see Fig. 1c). Actually this corresponded to variation of the grating period d, which is labelled on the abscissa in Fig. 5.

The main feature of photonic jets in hemispherical gratings, in contrast to DG types considered above, is a greater focal distance. As follows from Fig. 5b, the focal distance of the PNJ begins to increase actually linearly with the grating period. In a jet of the highest quality, produced by a HDG with a period $d = 4.7\lambda$, the maximal intensity is observed at the focal distance longer than 4λ from the grating surface. In this case, the PNJ length is $L = 6.6\lambda$, which is close to the corresponding value of the best (with respect to the parameter Q) jet from the RDG.

It is clear, that payment for such record parameters is not very good transverse localisation of the photonic jet. Generally, the values of the jet width R are the highest. The only exception is the limiting case of adjacent grooves ($D = 0$) when the photonic jet arises just on the groove edge and has a shape of an ellipse elongated in the direction of wave propagation with the minor axis length $R \approx \lambda/4$, which is the maximal spatial resolution obtained in our calculations. The intensity of such a jet is also maximal.

In increasing the separation between grating grooves to $R \approx \lambda/4$, the spatial profile of intensity within the limits of the focal volume becomes multimodal with noticeable side lobes (see Fig. 1c), and the PNJ itself loses its transverse localisation and is no longer sub-diffracting ($R > \lambda/2$).

3. Influence of a coating

Real DGs are usually coated with one or several thin layers of a material possessing, as a rule, physical-chemical properties different from those of the grating matrix. The main goal of the coating is, in addition to mechanical protection, to change the reflecting capability of the working surface. In phase gratings the coating is intended to maximally reduce or even suppress wave reflection (antireflection coatings), whereas in amplitude gratings, on the contrary, it is necessary to increase the reflection coefficient for the radiation passing to a DG. Obviously, an additional gradient of the refractive index on a

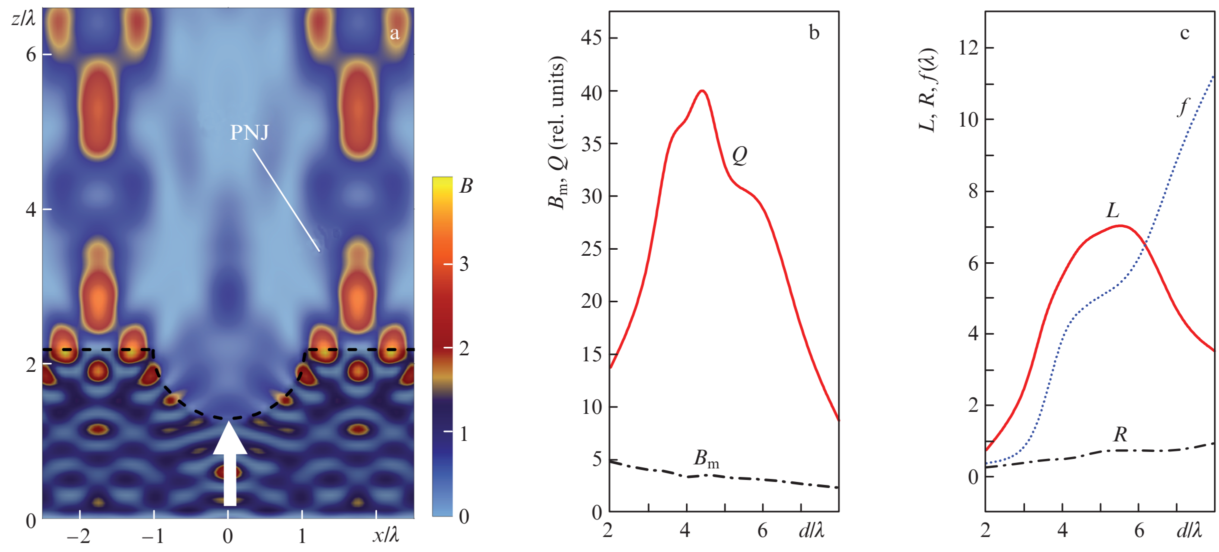

Figure 5. (Colour online) Same as in Fig. 3, for a HDG vs. the grating period.

grating surface affects the near-field characteristics and, consequently, PNJ parameters.

While studying the influence of the coating we limited ourselves to the grating with triangular grooves and the blaze angle $\alpha = 45°$ considered above. This configuration, as mentioned, provides the highest PNJ intensity. For the external coating in numerical simulation we chose magnesium fluoride (MgF_2) with the refractive index $n_c = \sqrt{\varepsilon_c} = 1.38$ at the considered wavelength of 532 nm and glass of the type of dense flint with a greater than in the DG refractive index $n_c = 1.7$. The first coating is antireflection ($\varepsilon_c < \varepsilon$), whereas the second coating is reflecting. Results of numerical simulation are presented in Fig. 6.

In Fig. 6a one can see a longitudinal distribution of the normalised optical intensity B in a photonic jet at a distance ξ calculated from the DG boundary (including the coating). For example, consider the case of the film coating with $l = \lambda/4$, which is the condition for the optimal antireflection effect. One can see that the optically less dense layer on the surface of the DG [curve (*2*)] results in an almost double peak intensity of the PNJ; the coating with a higher refractive index [curve (*3*)] reduces the intensity approximately twice. Meanwhile, in DGs with a coating and without it the spatial position of the intensity maxima in a jet is almost the same. This confirms that these maxima arise due to interference of fields from neighbouring grooves of the DG, i.e., are related to the periodicity of a scattering object structure rather than to optical properties of the grating groove itself.

Note that if the refractive index of the film is even greater than in Fig. 6a, then the peak intensity of the PNJ will be lower and at $n \geqslant 2$ the photonic jet from such a DG actually vanishes. The reason is the total reflection condition that is fulfilled on the external boundary of the coating for the light wave propagating through a triangular grating groove.

Dependences of the main parameters of the PNJ formed by a grating with triangular grooves on the coating width are

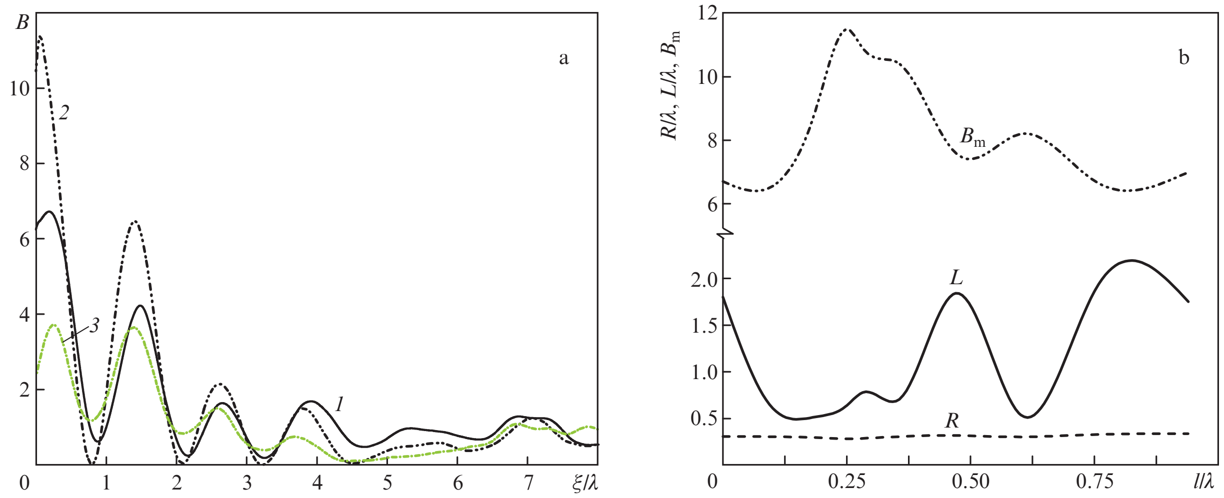

Figure 6. (a) Longitudinal profile of the PNJ intensity in the cases of a TDG without a coating (*1*) and with a coating of width $l = \lambda/4$ (*2*, *3*) for the refractive indices $n_c = 1.38$ (*2*) and 1.7 (*3*) and (b) the main parameters of the PNJ vs. the thickness of the coating with $n_c = 1.38$.

given in Fig. 6b. One can see that the coting on a grating substantially changes the photonic jet properties. In particular, a quarter-wave film, as mentioned above, noticeably increases the peak intensity of the PNJ, however, the jet length in this case sharply reduces and becomes comparable with a jet width. In other words, the spatial shape of the photonic jet changes from an elongated ellipse (in the transverse coordinates) to a circle. A similar but less pronounced effect is observed at the film width $l \approx 0.6\lambda$ as well. In changing l, the width of the PNJ remains virtually constant.

4. Conclusions

Using the numerical electrodynamical simulation of the near-field structure in light wave scattering on phase diffraction gratings of three geometrical types (with triangular, rectangular and hemispherical grooves) we have investigated characteristics of the domains with a high concentration of optical fields – photonic nanojets. The length, width, remoteness and intensity of arising PNJs have been studied. All the PNJ characteristics depend on the dimensional parameters of the gratings; this opens possibilities to control photonic jets by varying the period, degree of filling and groove profiles.

Each of the considered types of the DG can form a photonic jet array with unique characteristics. A PNJ from the grating with a triangular groove profile possesses the highest intensity. Rectangular grooves generate light fluxes with the best spatial localisation in the transverse direction and with moderate intensity. The most distant (from the grating surface) and simultaneously sufficiently long PNJs are formed by gratings with a hemispherical profile of grooves.

The influence of an external optically contrast coating of the DG is revealed in an additional modulation of the PNJ intensity due to wave interference inside the film, which, at certain values of the coating thickness, increases the peak intensity of the jet and simultaneously reduces the jet length.

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