Прохождение рентгеновского пучка через двумерный фотонный кристалл и эффект Тальбота

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Transmission of an X-ray beam through a two-dimensional photonic crystal and the Talbot effect

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Keywords: X-ray transmission; two-dimensional photonic crystal; Talbot effect; computer simulations; iterative algorithm.

Results of computer simulations of the transmission of an X-ray beam through a two-dimensional photonic crystal as well as the propagation of an X-ray beam in free space behind the photonic crystal are reported. The photonic crystal consists of a square lattice of silicon cylinders of diameter 0.5 μm. The amount of matter in the path of the X-ray beam rapidly decreases at the sides of the cylinder projections. Therefore the transmission is localized near the boundaries, and appears like a channeling effect. The iterative method of computer simulations is applied. This method is similar to the multi-slice method that is widely used in electron microscopy. It allows a solution to be obtained with acceptable accuracy. A peculiarity in the intensity distribution inside the Talbot

Как увидеть нано-объекты ?

ПЗС (CCD, charge-couple device) детекторы

имеют размер пиксела 25 мкм и больше.

Рентген подается на флуоресцентную пленку, толщина < 1 мкм

Пленка конвертирует рентген в видимый свет

Оптика (линзы) увеличивает до 50 раз (стандартно 20 раз)

В результате получаем размер пиксела < 1 мкм

Но разрешение такого детектора не лучше, чем 1 мкм

Период фотонного кристалла 0.5 мкм (500 нм) и меньше !

Не хватает ! Решение:

Рентгеновские линзы могут увеличить еще в 20 раз

Только в этом случае можно что-то увидеть.

Рентгеновский микроскоп **реально** дает новые возможности

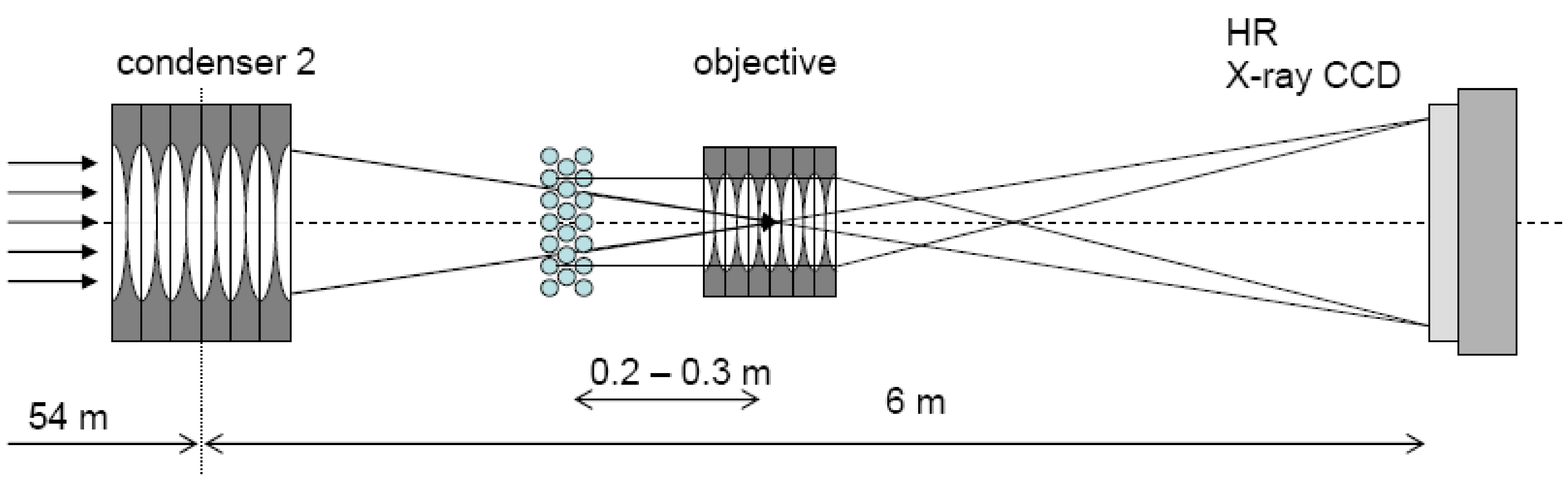
Это не игрушка, поиграли и бросили.

Some CRL applications. **High resolution x-ray 2D microscopy**. Snigirev et al. with Lengeler's CRLs

(1) – The object is illuminated through a CRL with a large aperture to condense the beam at the object area under illumination (condenser 2)

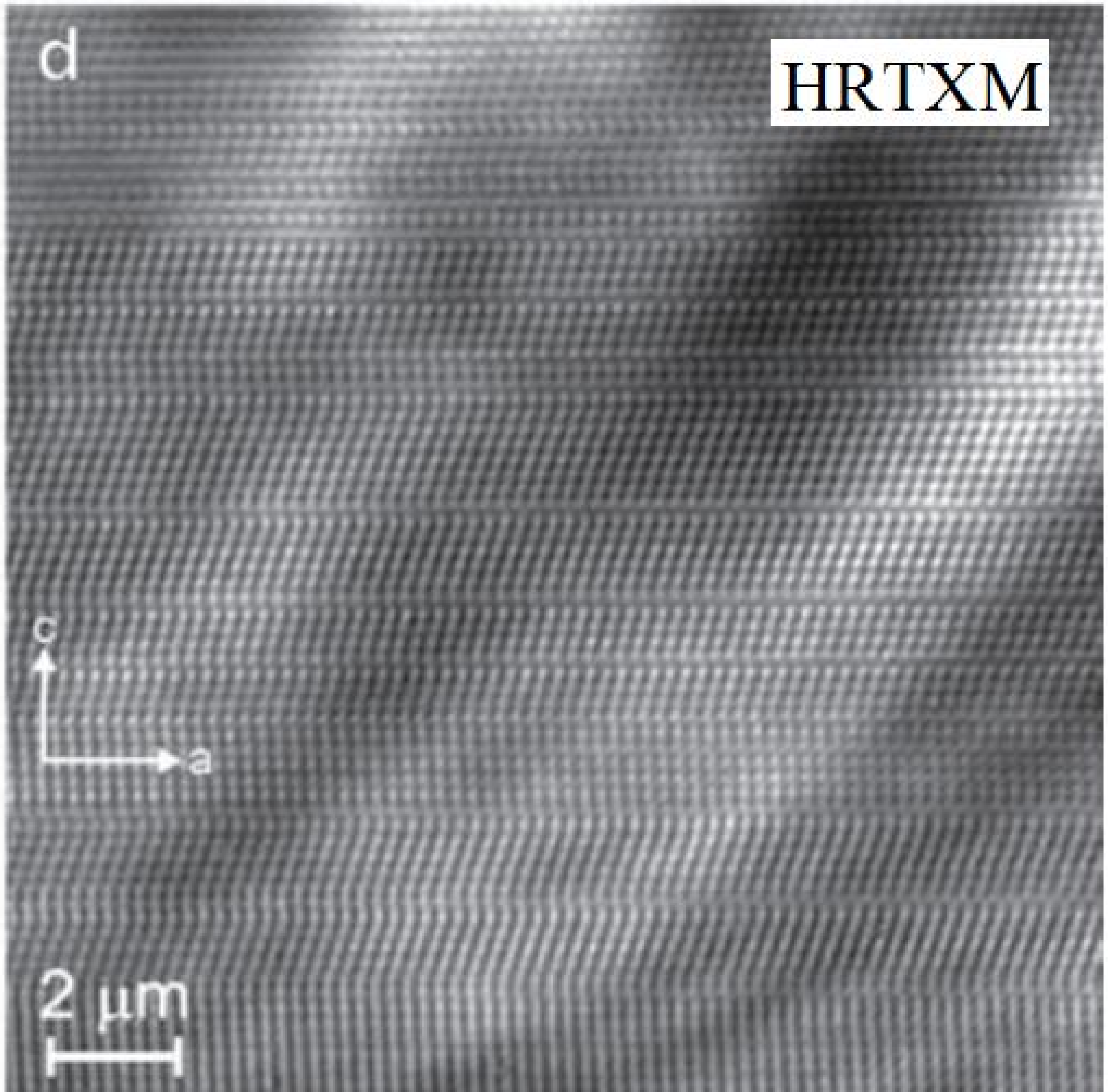
(2) – Objective CRL (objective) has a short focus length and it works as a microscop. Large magnification is necessary to adjust CCD detector resolution (about $1\ \mu m$)

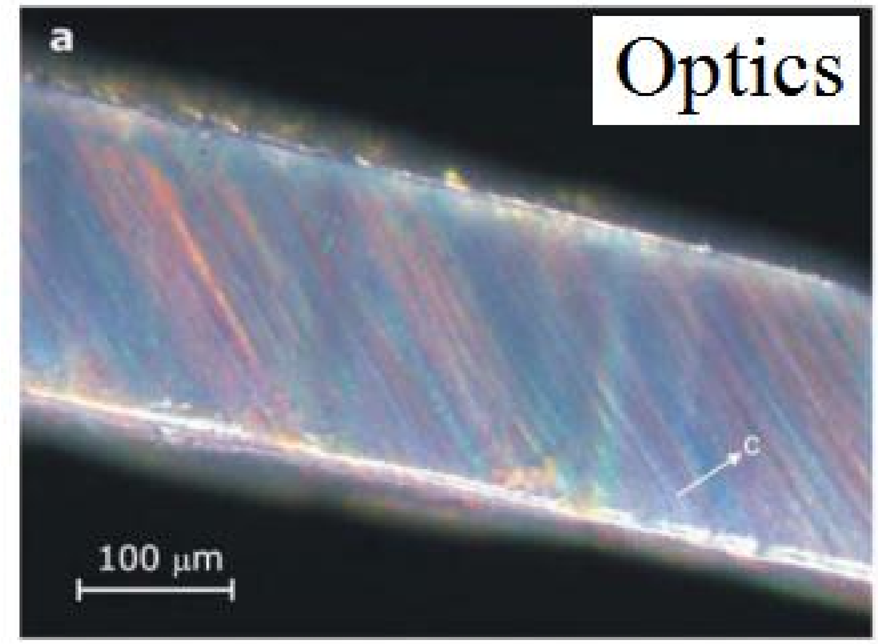
This technique allows one to see a real structure of opal crystals and photon crystals. The theory is not developed

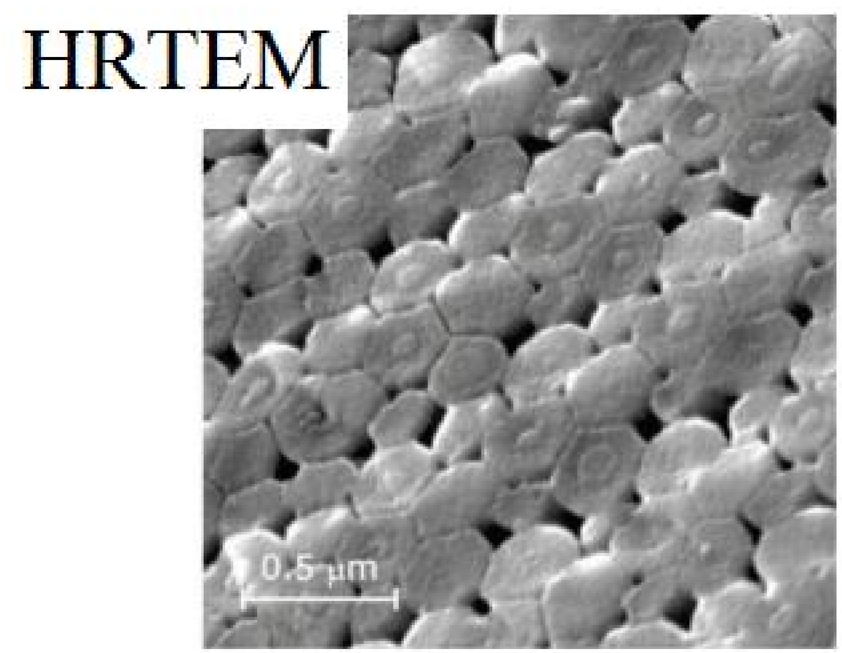


High-Resolution Transmission X-ray Microscopy: A New Tool for Mesoscopic Materials (Natural opal)

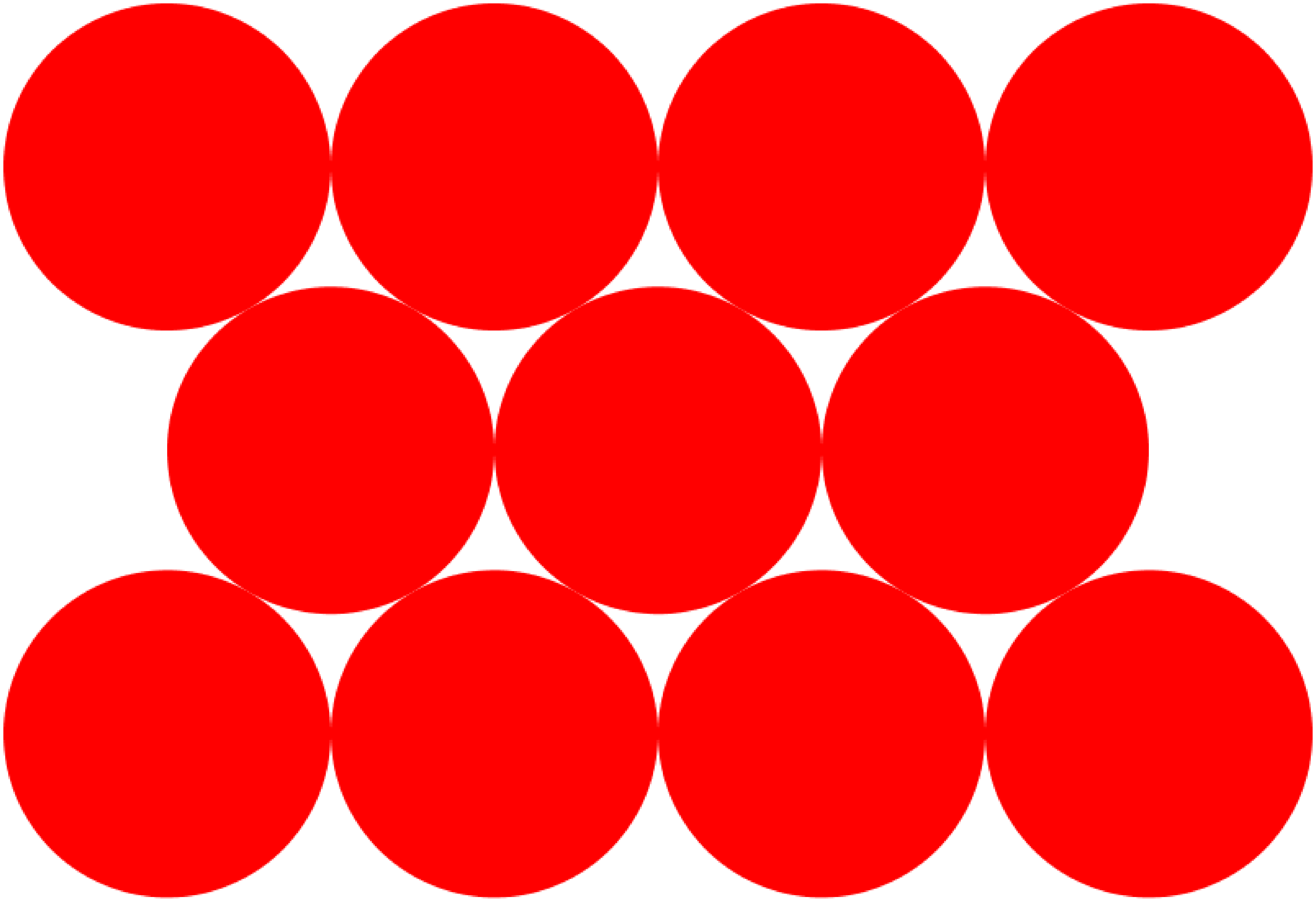
By *Alexey Bosak, Irina Snigireva,* Kirill S. Napolskii,* and *Anatoly Snigirev*

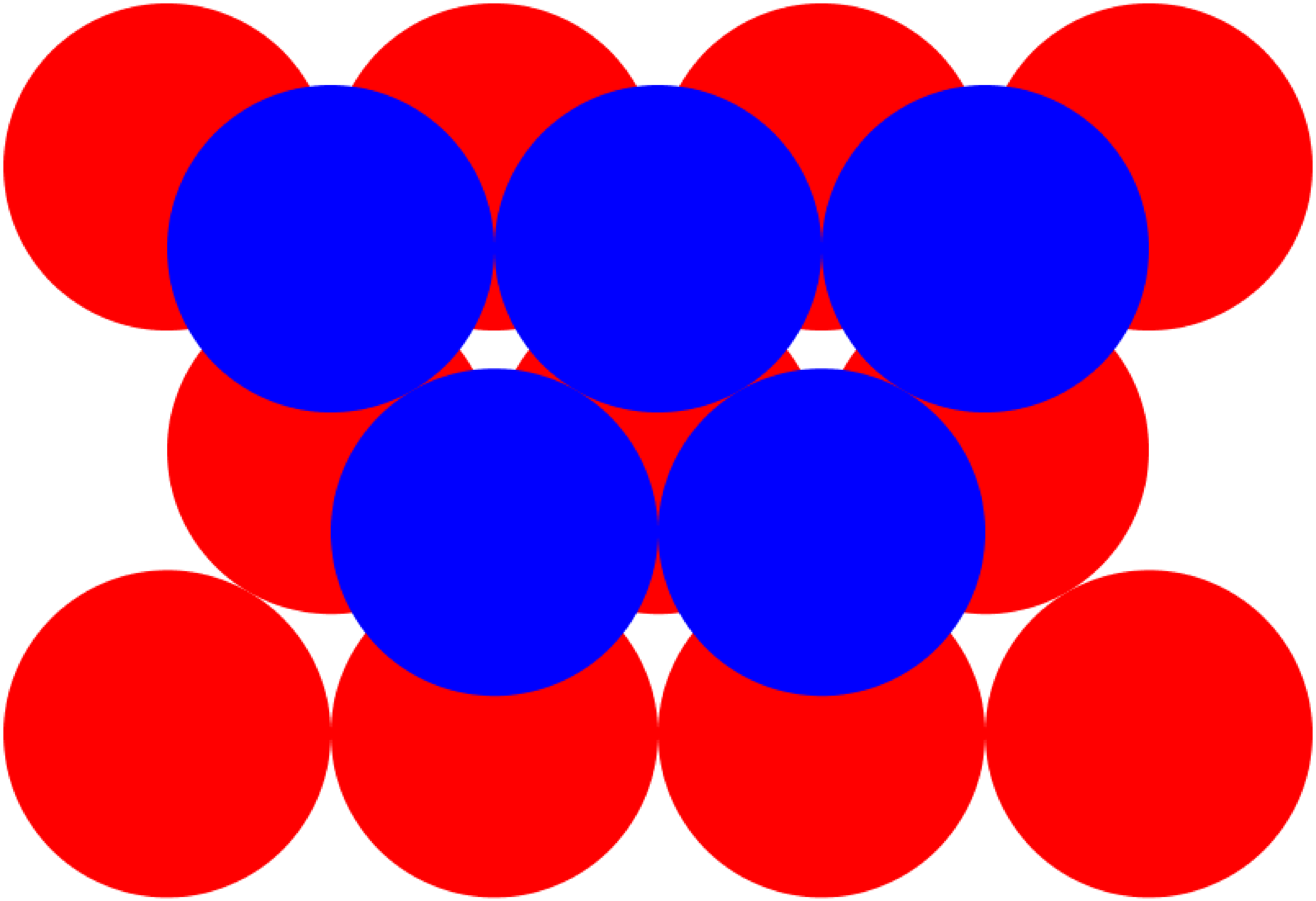




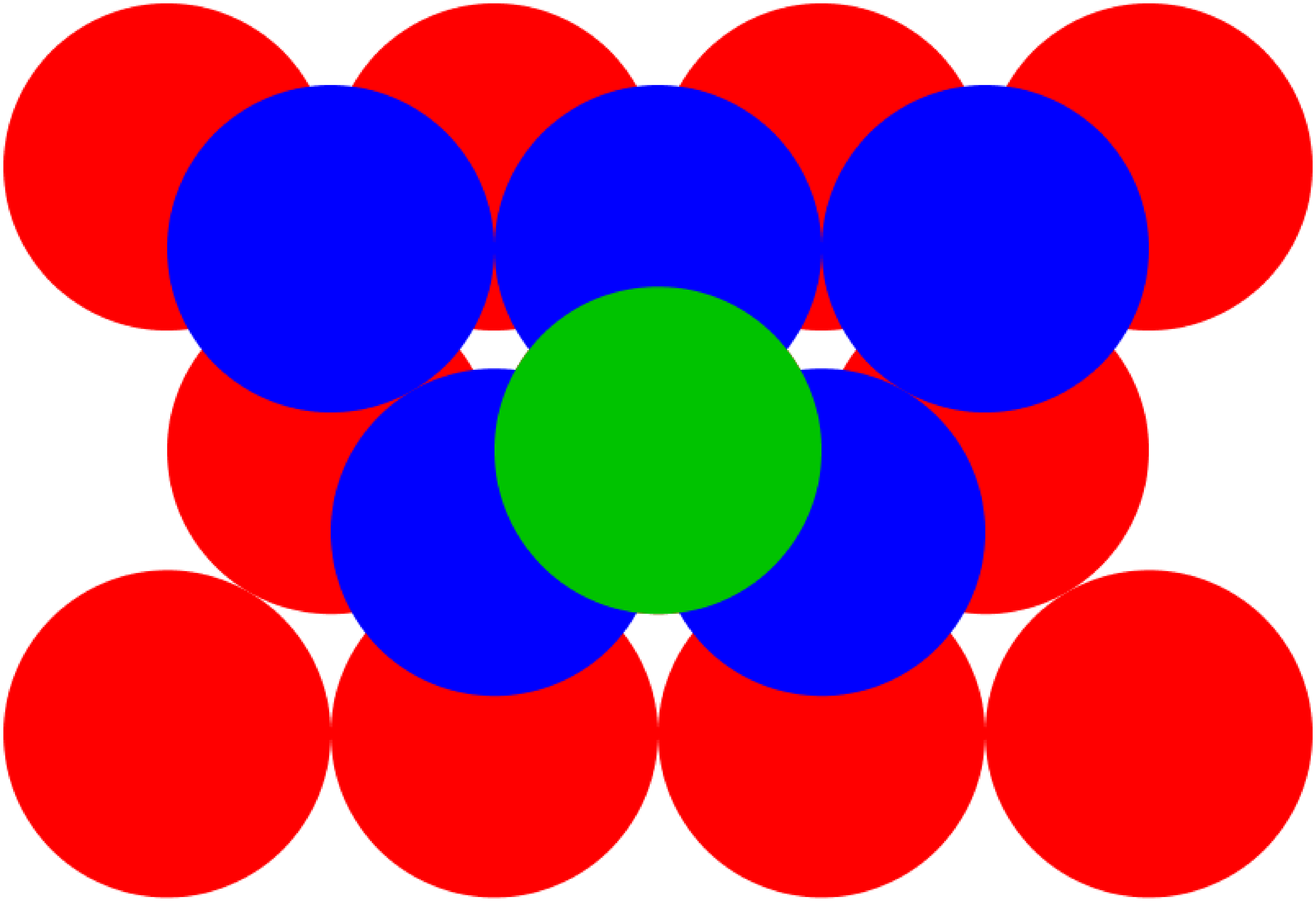


Adv. Mater. **2010**, *22*, 3256–3259

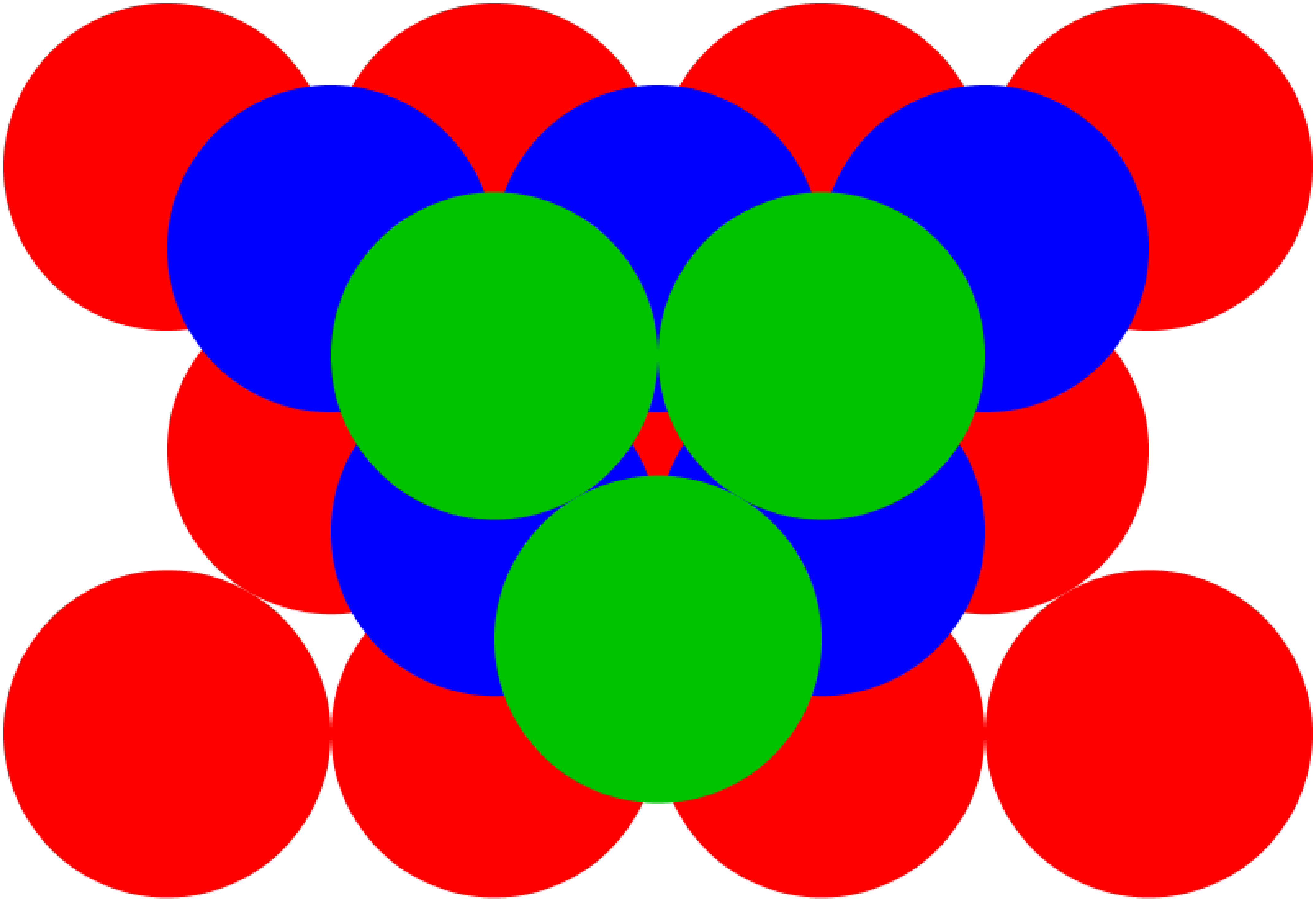




ГПУ решетка, имеет сквозные каналы



ГЦК решетка, 111 направление



История вопроса, 1-я статья, 3D и все в кристалле

КРИСТАЛЛОГРАФИЯ, 2014, том 59, № 1, с. 5–10

ДИФРАКЦИЯ И РАССЕЯНИЕ ИОНИЗИРУЮЩИХ ИЗЛУЧЕНИЙ

УДК 548.73

ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ ИЗОБРАЖЕНИЙ ФОТОННЫХ КРИСТАЛЛОВ С ПОМОЩЬЮ ЖЕСТКИХ РЕНТГЕНОВСКИХ ЛУЧЕЙ В СХЕМЕ НА ПРОСВЕТ. БЛИЖНЕЕ ПОЛЕ

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Поступила в редакцию 03.04.2013 г.

Развит метод расчета прохождения жесткого рентгеновского излучения через идеальный и хорошо ориентированный фотонный кристалл, состоящий из плотно упакованных сфер вещества. Метод основан на использовании приближенного решения параксиального уравнения на малых расстояниях. Получена рекуррентная формула для распространения излучения на один период кристалла. Разработана компьютерная программа для численного моделирования изображений фотонных кристаллов в ближнем поле, в частности сразу за кристаллом. Расчет выполнен для силикатных сфер диаметром 500 нм. Показано, что метод стандартного фазового контраста не применим к данным объектам, так как в объеме кристалла происходит весьма сильное изменение интенсивности, обусловленное рассеянием излучения на отдельных сферах.

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История вопроса, 1-я статья, результаты

Для практической реализации описанного метода расчета рассмотрен фотонный кристалл, состоящий из сфер SiO_2 диаметром D и имеющий структуру типа *ABABAB*. Направление пучка (ось z) совпадает с осью гексагональной симметрии. Период кристалла по оси z равен $h = D(8/3)^{1/2}$. На рис. 1 показана функция $s(x,y)$ в виде черно-бело-

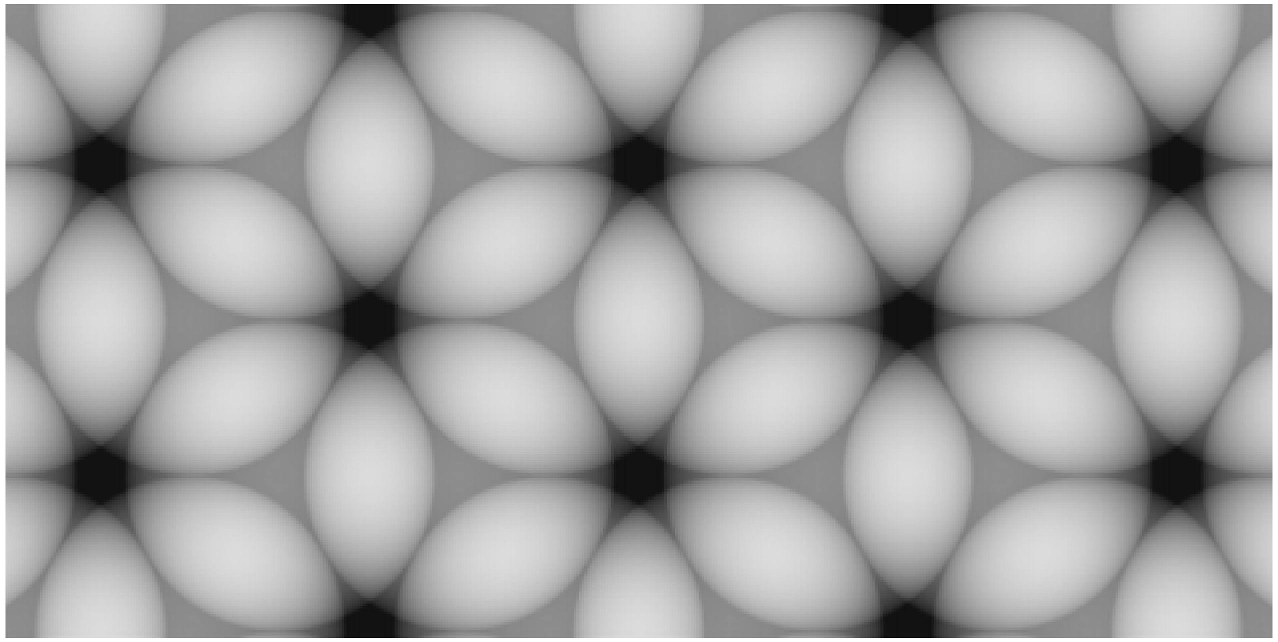

Рис. 1. Функция $s(x, y)$ на расчетной области.

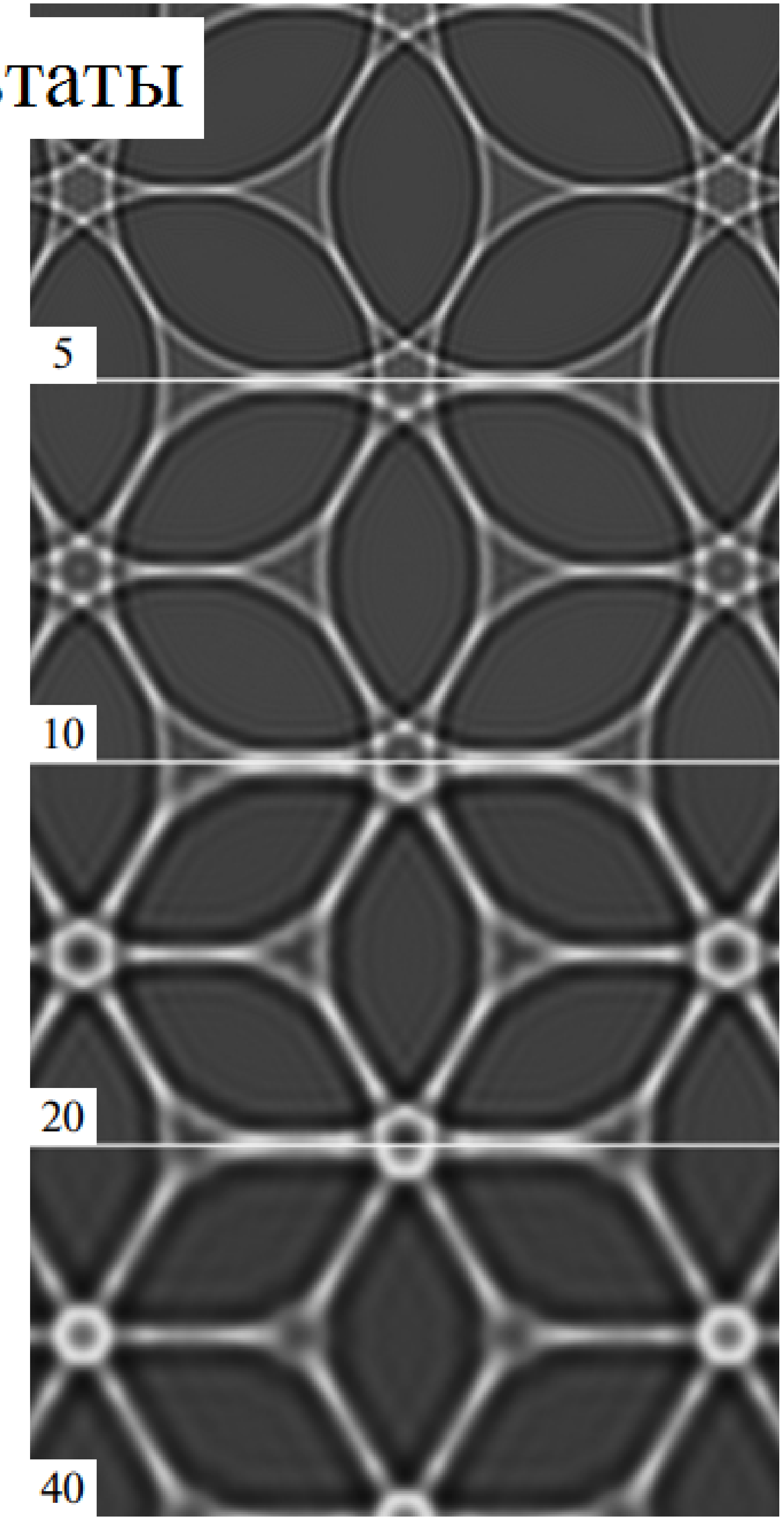

Рис. 2. Карты распределения интенсивности излучения для разных толщин кристалла. Толщина измеряется числом периодов, которое показано на панелях.

История вопроса, 2-я статья, 3D и за кристаллом

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Propagation of an X-ray beam modified by a photonic crystal

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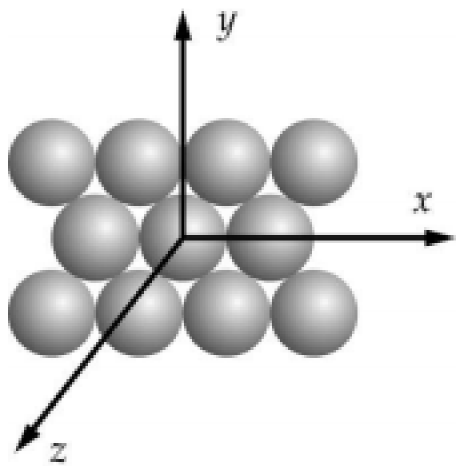
A method of calculating the transmission of hard X-ray radiation through a perfect and well oriented photonic crystal and the propagation of the X-ray beam modified by a photonic crystal in free space is developed. The method is based on the approximate solution of the paraxial equation at short distances, from which the recurrent formula for X-ray propagation at longer distances is derived. A computer program for numerical simulation of images of photonic crystals at distances just beyond the crystal up to several millimetres was created. Calculations were performed for Ni inverted photonic crystals with the [111] axis of the face-centred-cubic structure for distances up to 0.4 mm with a step size of 4 µm. Since the transverse periods of the X-ray wave modulation are of several hundred nanometres, the intensity distribution of such a wave is changed significantly over the distance of several micrometres. This effect is investigated for the first time.

История вопроса, 2-я статья, результаты



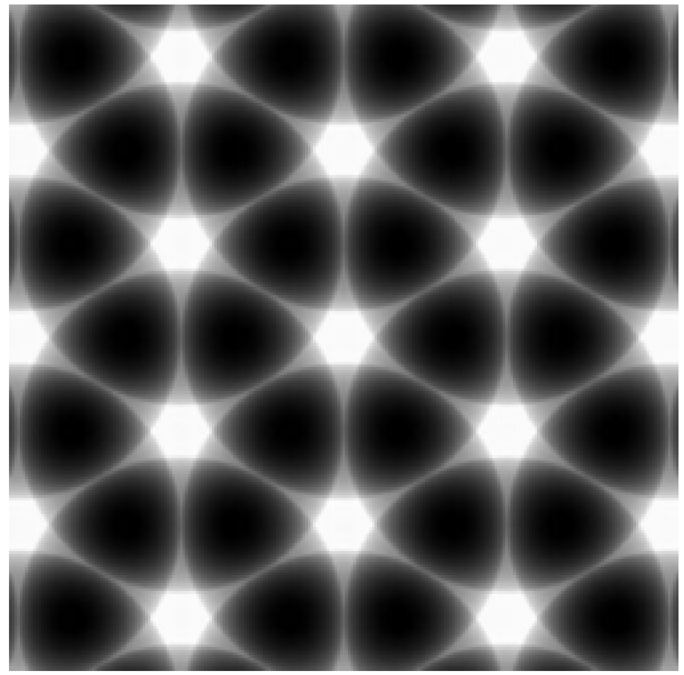


Figure 2
The function $s(x, y)$ within the calculating area. See text for details.

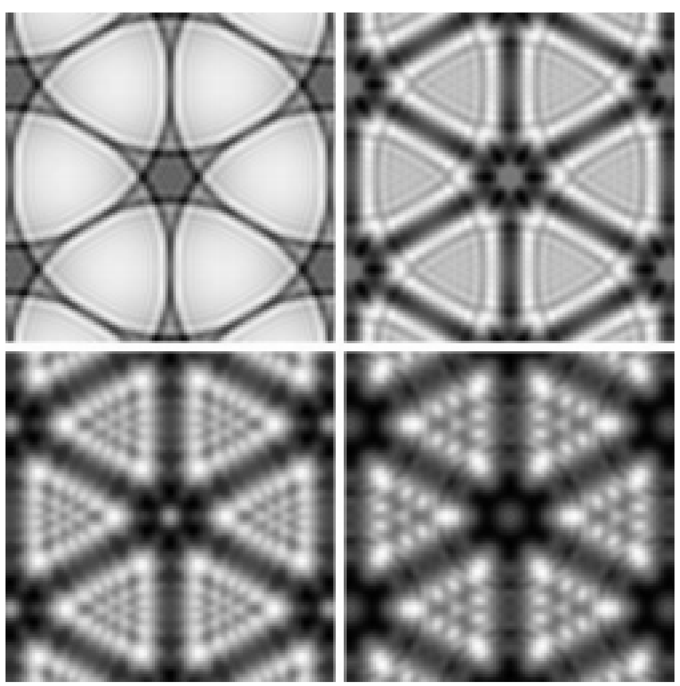


Figure 3
Intensity distributions at distances 0, 8, 16 and 24 µm. The images are ordered from left to right and from top to bottom.

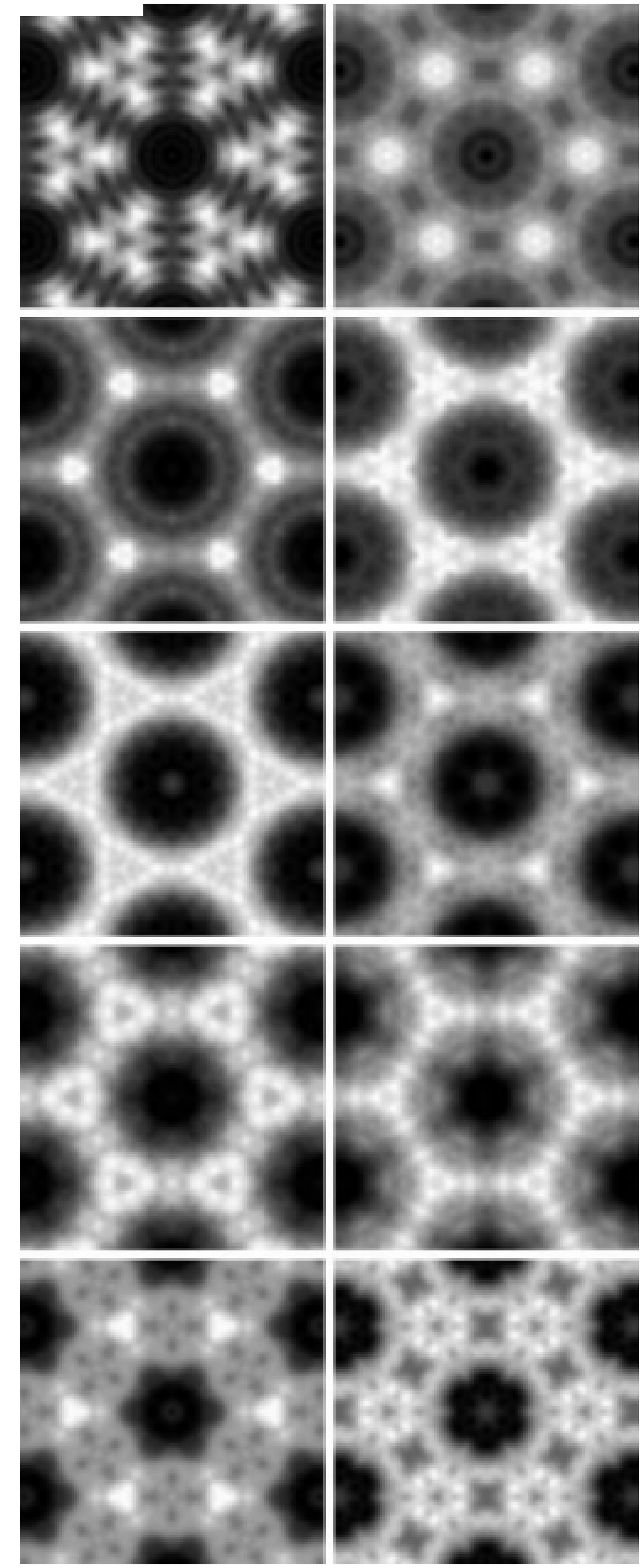


Figure 5
Intensity distributions at distances from 40 µm to 400 µm with a step of 40 µm. The images are ordered from left to right and from top to bottom. See text for details.

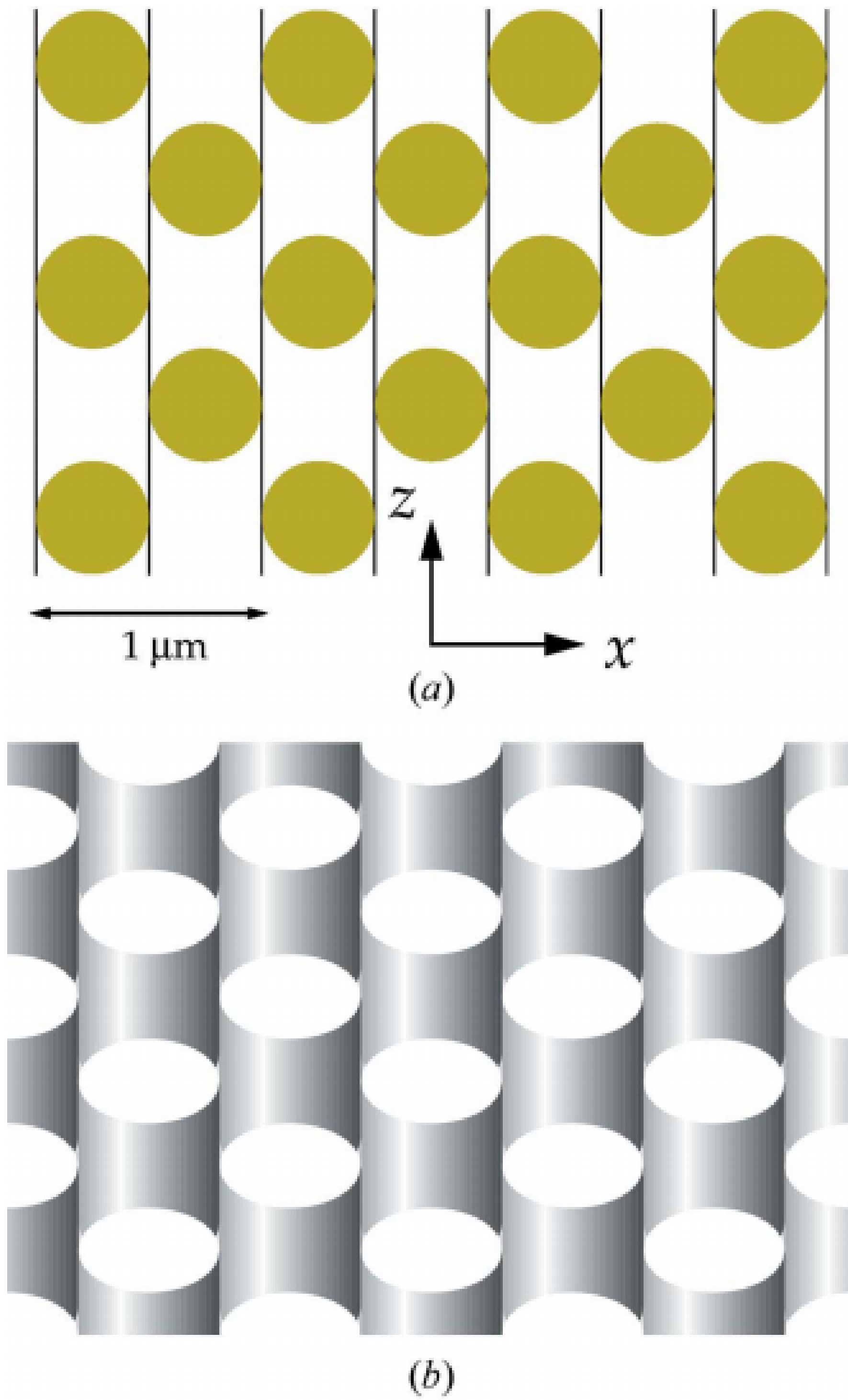


Figure 1
Structure of the two-dimensional photonic crystal used here in the computer simulations. (*a*) View from the top and (*b*) the three-dimensional picture.

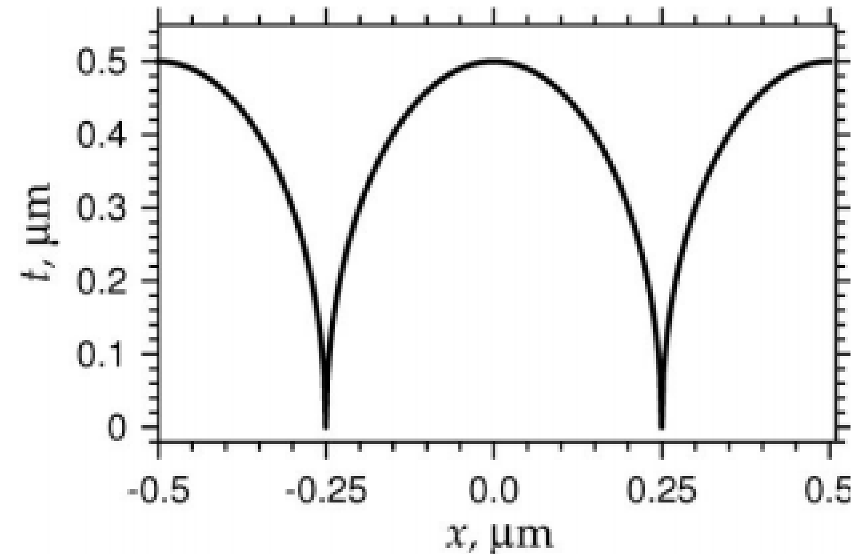


Figure 2
A profile of thickness t of Si matter averaged over a period along the beam direction.

In recent works (Kohn & Tsvigun, 2014; Kohn *et al.*, 2014) an iterative approach based on recurrence relations has been proposed. It is similar to the multi-slice method used in the theory of transmission electron microscopy [see Goodman & Moodie (1974), and references therein], but not entirely. Our method is valid only for periodic systems, *i.e.* for the case where the region of three periods can be calculated in each iteration and the side periods are improved to be equal to the central period. This method was applied to three-dimensional photonic crystals. In this work we apply the same approach to the two-dimensional photonic crystal shown in Fig. 1 for a special orientation of the crystal relative to the beam direction which is shown in Fig. 1(*a*) as the z-axis.

This case is of interest due to the existence of the channeling effect for part of the X-ray beam. A profile of thickness t of Si matter averaged over a period along the beam direction is shown in Fig. 2. The argument is the transverse coordinate x. It shows two minima on the x-axis at the boundaries of the cylinders. These minima have a square-root dependence. It is known that for the focusing lens the minimum has a parabolic profile.

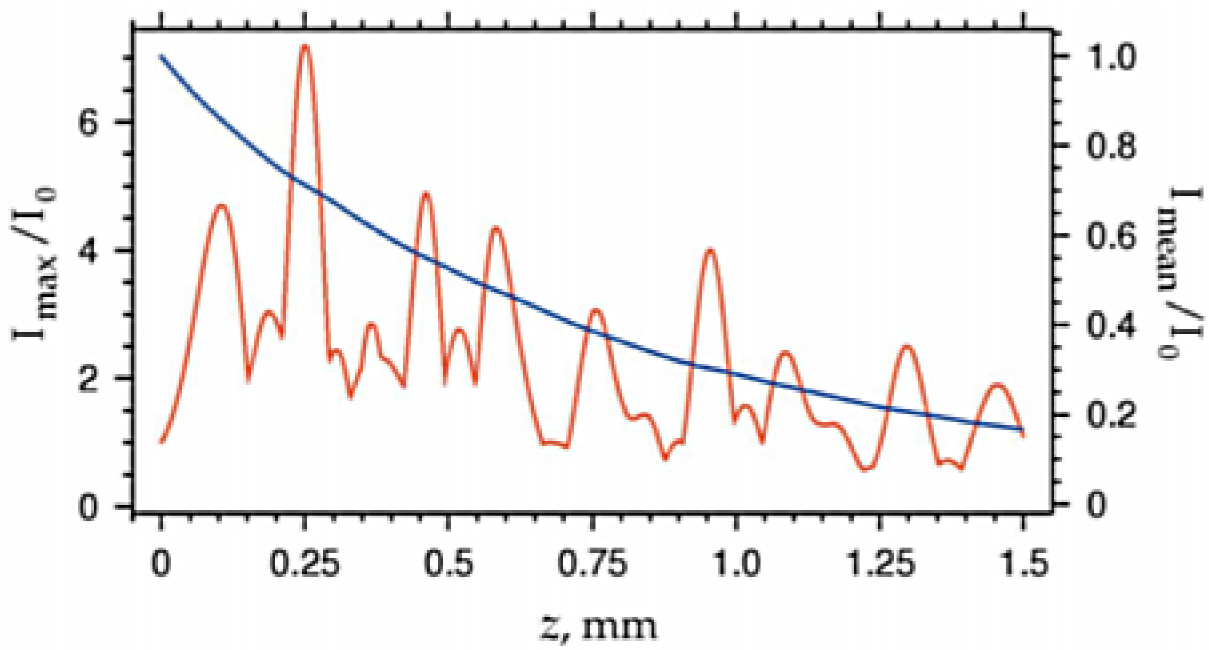


Figure 4
Dependence of the maximum value of the X-ray beam intensity (red curve, left-hand axis) and mean value (blue curve, right-hand axis) on the thickness of the photonic crystal.

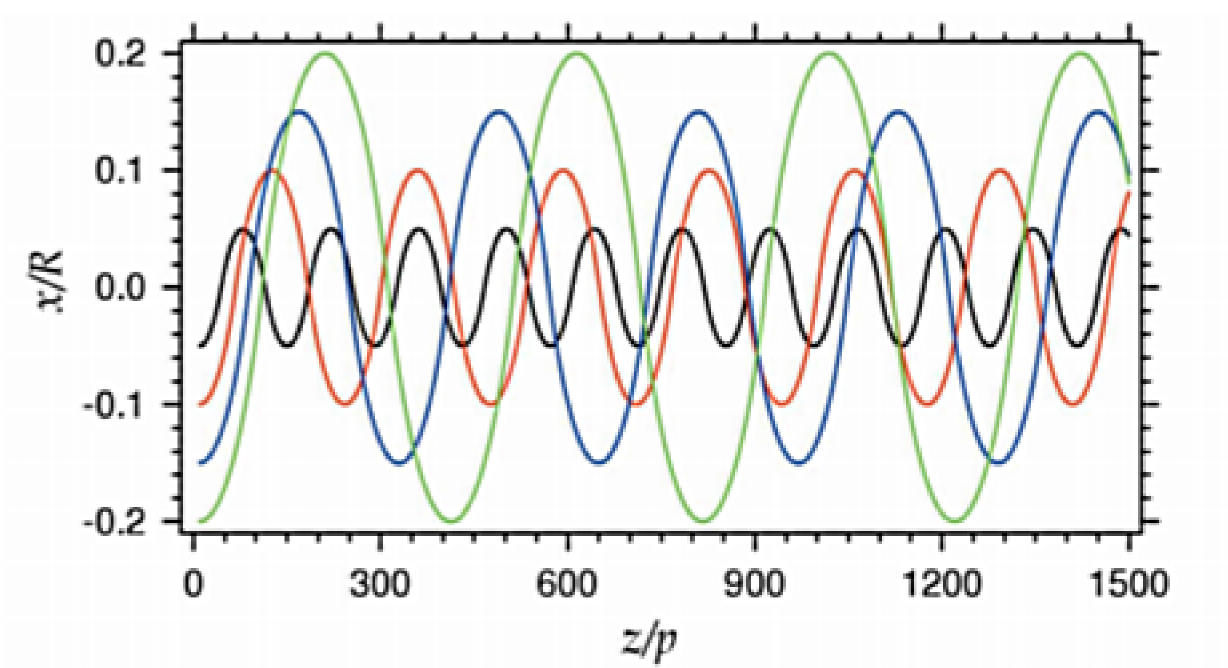


Figure 5
Ray trajectories in the geometrical optics approximation. Four lines with various initial positions are drawn with various colors to better distinguish them.

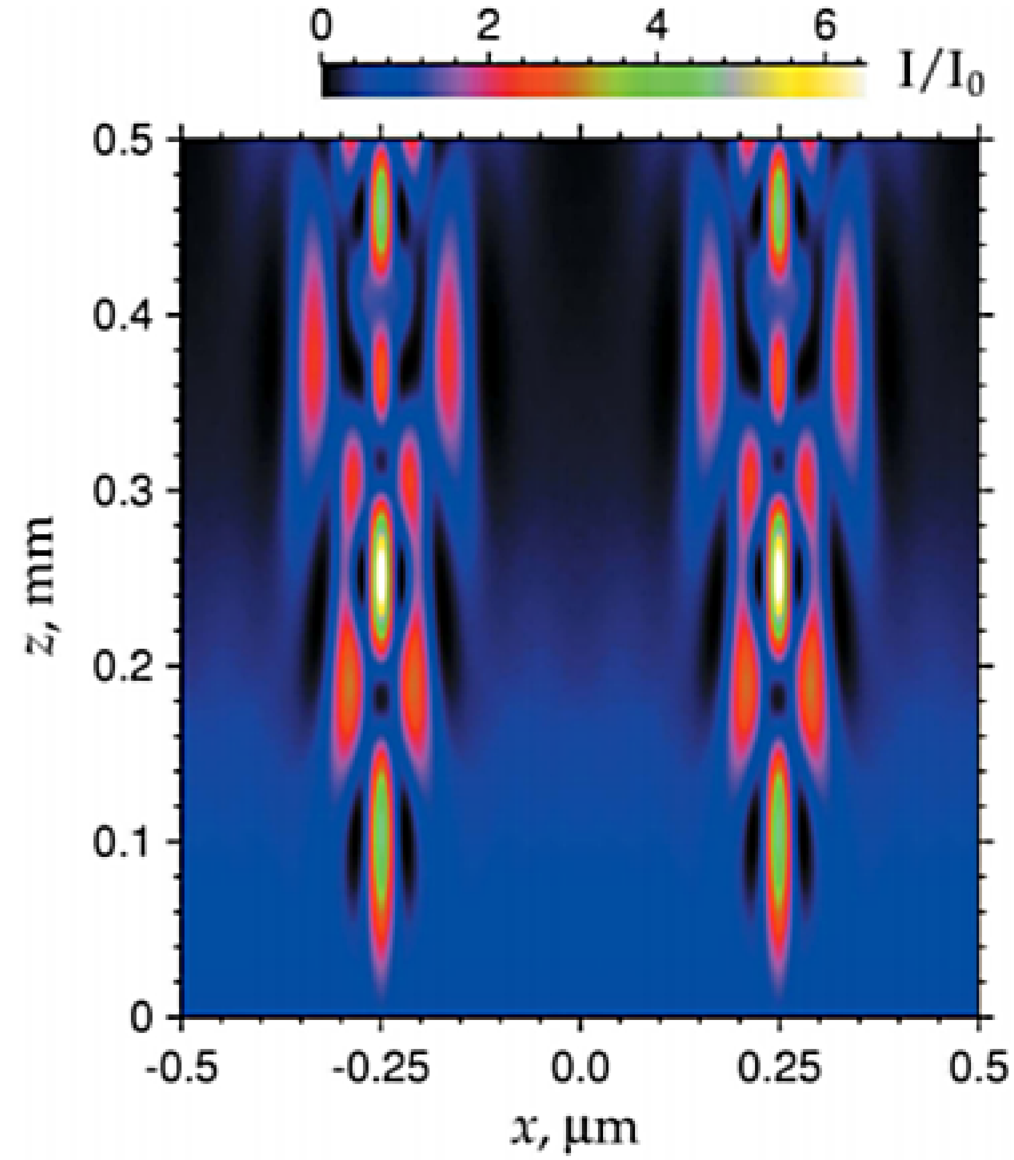


Figure 3
X-ray beam intensity distribution inside the photonic crystal.

arity in equation (17), introduce dimensionless variables $s = x/R$ and $n = z/p$, and obtain the following equation for the ray trajectory in the case of an incident plane wave,

$$\frac{d^2 s}{dn^2} = -u(s), \qquad \frac{ds(0)}{dn} = 0, \qquad s(0) = s_0, \tag{18}$$

where

$$u(s) = (32)^{1/2}\,\delta\,\frac{s|s|^{1/2}}{(s^2 + a^2)}\left(1 - \frac{|s|}{2}\right)^{-1/2}(1 - |s|). \tag{19}$$

Here, a is a small parameter which is necessary for computer calculations without a singularity. In reality the approach of

Эффект Тальбота и странная особенность

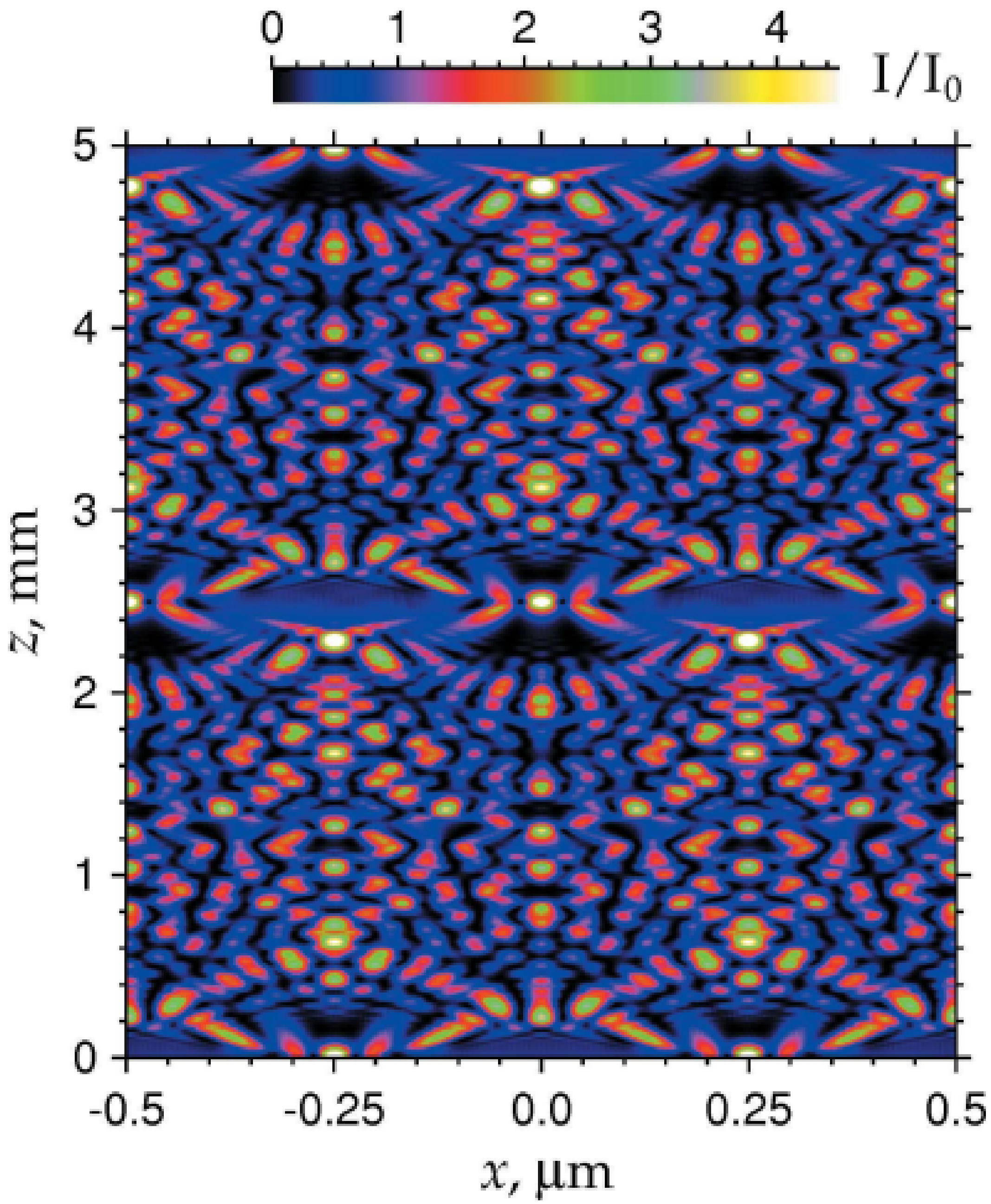
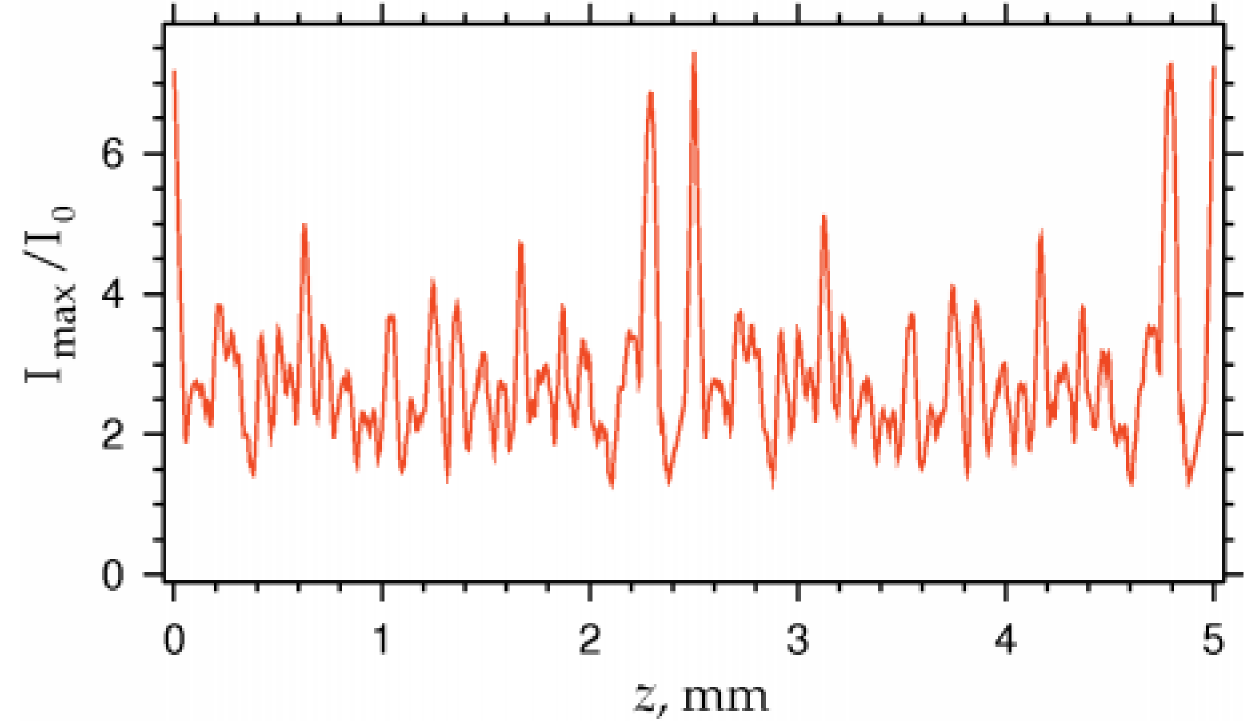


Figure 6
X-ray beam intensity distribution behind the photonic crystal within the Talbot period.



$$\psi(x,0)=\sum_m C_m \exp(iq_m x), \quad q_m = 2\pi\frac{m}{p}$$

$$\psi(x,z)=\sum_m C_m \exp\left(2\pi i\left[\frac{x}{p}m-\frac{z}{z_T}m^2\right]\right), \quad z_T=\frac{2p^2}{\lambda}$$

$$\psi(x,z_T+z)=\psi(x,z) \qquad \psi(x,\frac{z_T}{2}+z)=\psi(x-\frac{p}{2},z)$$

Если $\mathrm{Im}(C_m)=0$, *то*

$$I(x,z_T-z)=I(-x,z),\ \ I(x)=|\psi(x)|^2$$

Эффект Тальбота и обнуление фазы начальной функции

Для новой функции $\psi'(x,0) = |\psi(x,0)|$

выполняется условие $I(x, z_T - z) = I(x, z)$

и приблизительно наблюдается дробный

эффект Тальбота, а именно, $I(x, \frac{z_T}{2n})$

имеет период в n раз меньше, то есть $\frac{p}{n}$

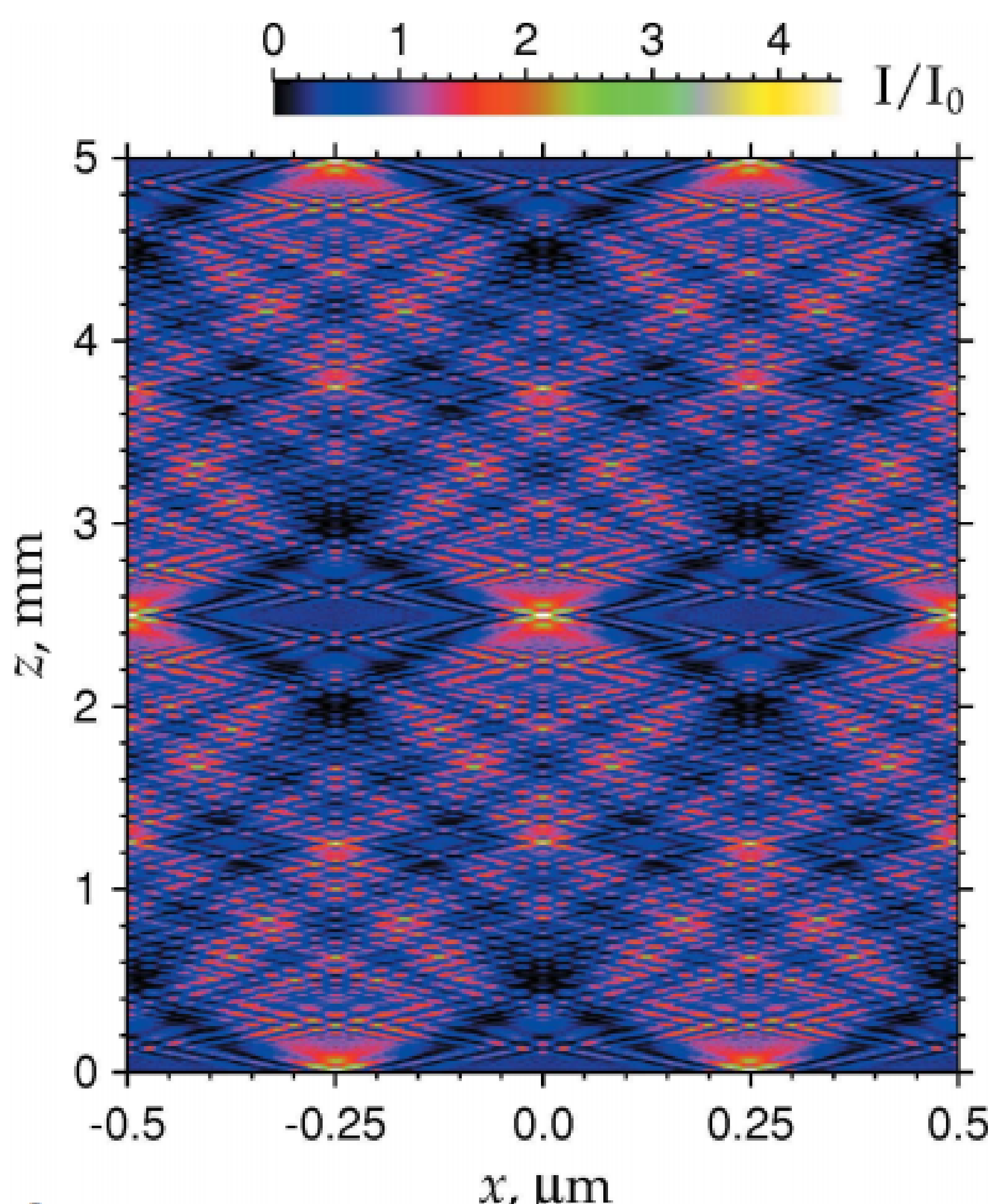
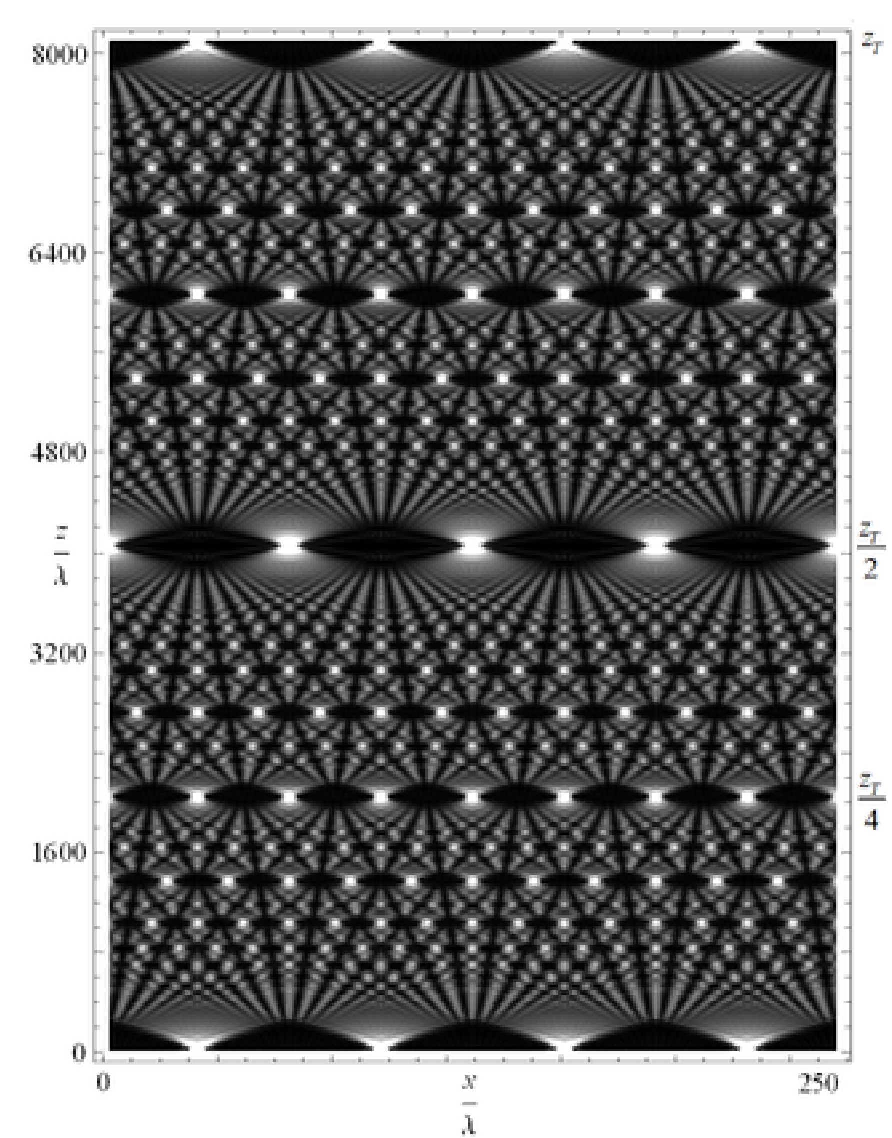


Figure 8
X-ray beam intensity distribution behind the photonic crystal within the Talbot period for the case of a wavefunction with initial modulus and zero phase.



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Caustics, multiply reconstructed by Talbot interference

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(*Received 27 August 1998*)

Abstract. In planar geometrical optics, the rays normal to a periodically undulating wavefront curve W generate caustic lines that begin with cusps and recede to infinity in pairs; therefore these caustics are not periodic in the propagation distance z. On the other hand, in paraxial wave optics the phase diffraction grating corresponding to W gives a pattern that is periodic in z, the period for wavelength λ and grating period a being the Talbot distance, $z_T = a^2/\lambda$, that becomes infinite in the geometrical limit. A model where W is sinusoidal gives a one-parameter family of diffraction fields, which we explore with numerical simulations, and analytically, to see how this clash of limits (that wave optics is periodic but ray optics is not) is resolved. The geometrical cusps are reconstructed by interference, not only at integer multiples of z_T but also, according to the fractional Talbot effect, at rational multiples of $z = z_T p/q$, in groups of q cusps within each grating period, down to a resolution scale set by λ. In addition to caustics, the patterns show dark lanes, explained in detail by an averaging argument involving interference.

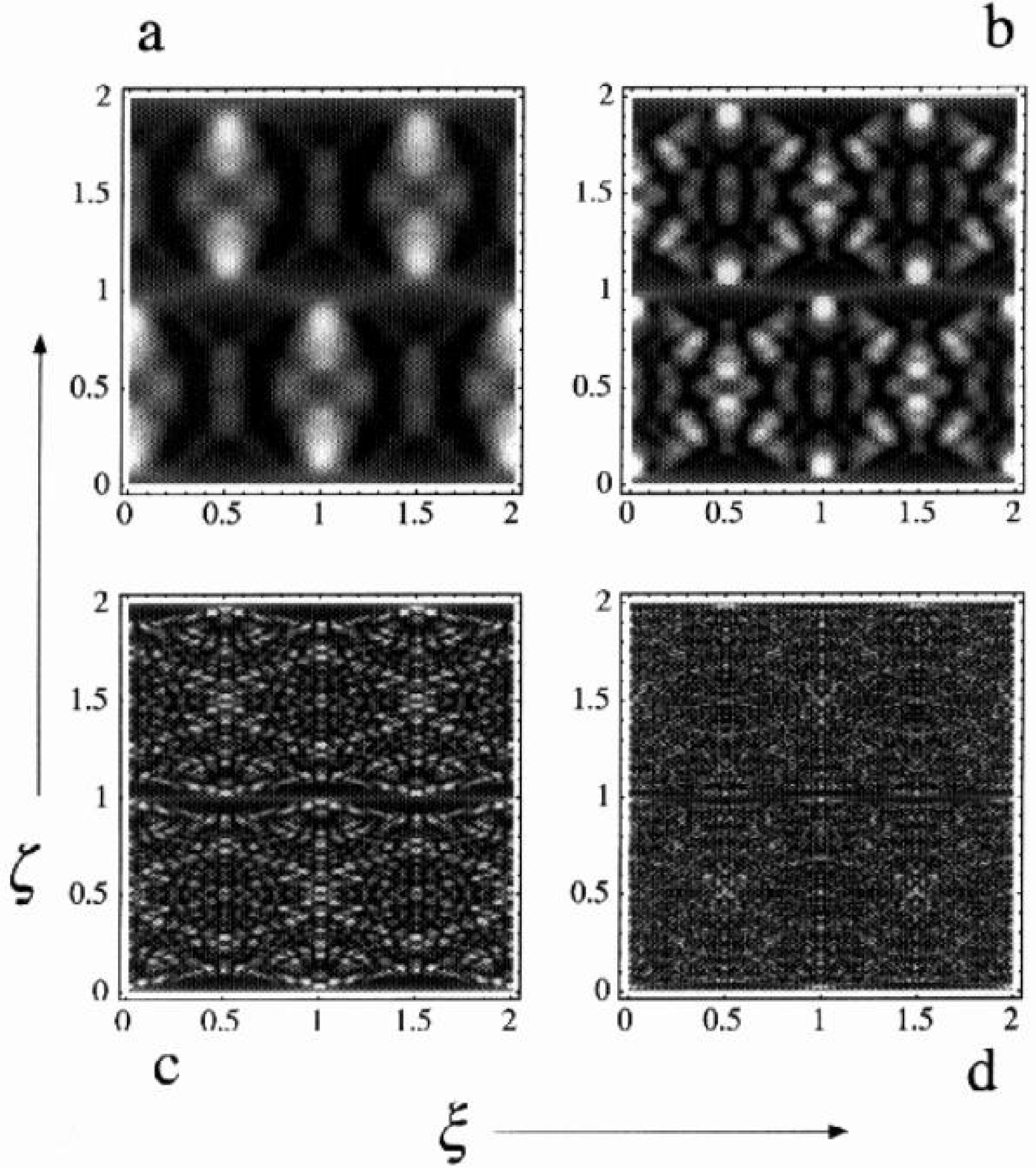

Figure 2. Density plots of Talbot phase-grating diffraction intensity $I = |\Psi|^2$,

Формулы теории и итерационный метод расчета

$$E(x, z, t) = \exp(ikz - i\omega t)\, A(x, z).$$

$$\frac{\partial A}{\partial z} = -ik\eta\, \rho(x, z)\, A + \frac{i}{2k}\frac{\partial^2 A}{\partial x^2}.$$

$$B_n(x) = A_n(x)\, C_1(x), \qquad C_1(x) = \exp\left[-ik\eta\, t_1(x)\right],$$

$$t_1(x) = \int_0^d \mathrm{d}z\, \rho_1(x, z).$$

$$t_1 = 0 \qquad \text{for } |x| < R,$$
$$t_1 = d\left[1 - (x-d)^2/R^2\right]^{1/2} \qquad \text{for } |x - d| < R,$$

$$A_{n+1}(x) = \int \mathrm{d}x_1\, P(x - x_1, d)\, B_n(x_1),$$

$$P(x, z) = \frac{1}{(i\lambda z)^{1/2}} \exp\left(i\pi \frac{x^2}{\lambda z}\right)$$

Формулы теории и итерационный метод расчета

$$B_{n+1}(x) = A_{n+1}(x)\,C_2(x), \quad C_2(x) = \exp\left[-ik\eta t_2(x)\right],$$

$$t_2(x) = \int_0^d \mathrm{d}z\, \rho_2(x, z).$$

$$t_2 = d(1 - x^2/R^2)^{1/2} \qquad \text{for } |x| < R,$$
$$t_2 = 0 \qquad \text{for } |x - d| < R.$$

$$A_{n+2}(x) = \int \mathrm{d}x_1\, P(x - x_1, d)\, B_{n+1}(x_1).$$

We have solved this problem as described below. The calculations were performed in an interval of 3 μm with the number of points 16384 = 2^{14}. This interval contains three large periods of 1 μm. This is equivalent to a situation where

Формулы теории и итерационный метод расчета

$$B_n(x) = A_n(x)\, C_1(x)\, C_2(x)$$

$$A_{n+2}(x) = \int \mathrm{d}x_1\, P(x - x_1, 2d)\, B_n(x_1).$$

$$A(x, z + z_0) = \int \mathrm{d}x_1\, P(x - x_1, z_0)\, A(x_1, z)$$

Б Л А Г О Д А Р Ю

З А

В Н И М А Н И Е