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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.

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

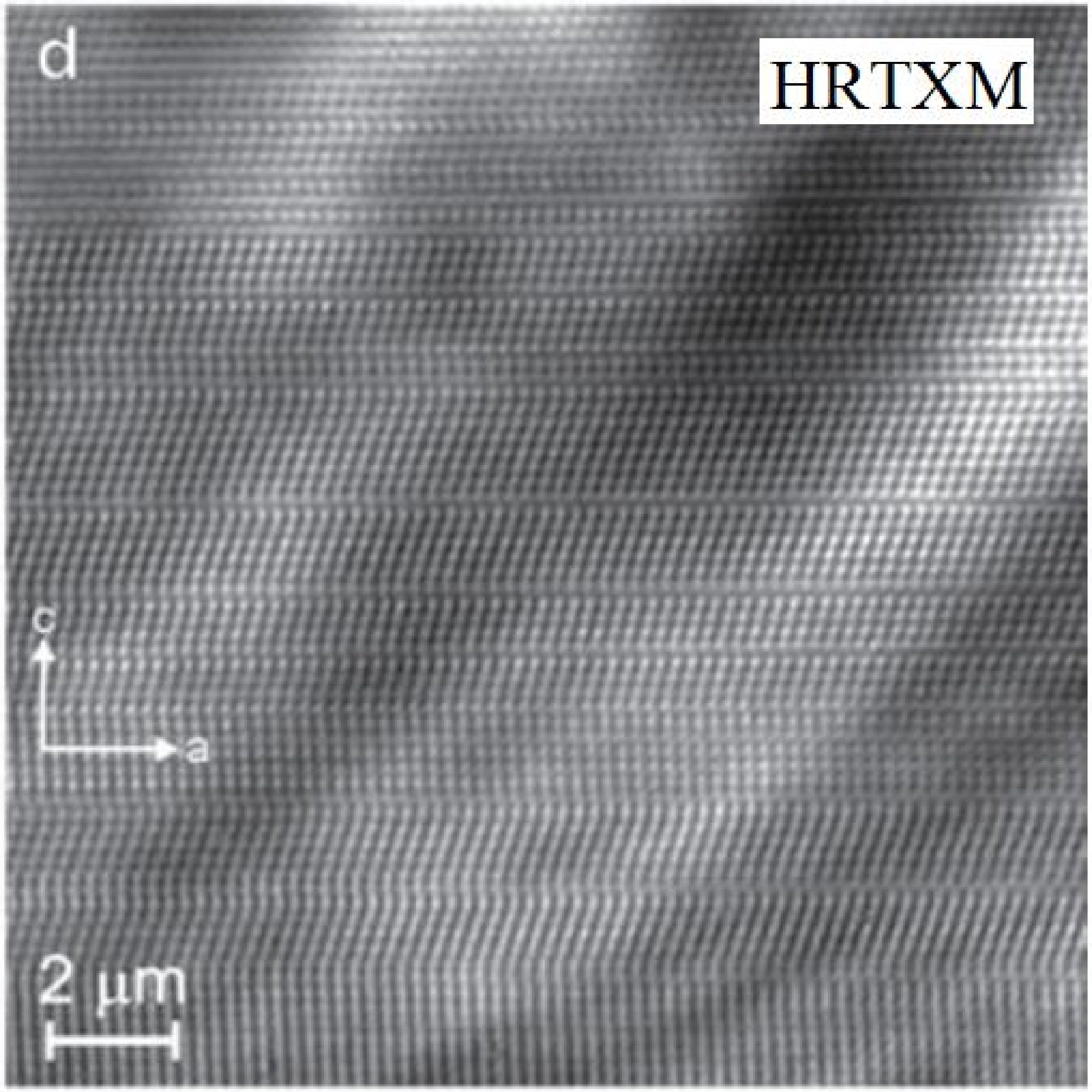
Только в этом случае можно что-то увидеть.

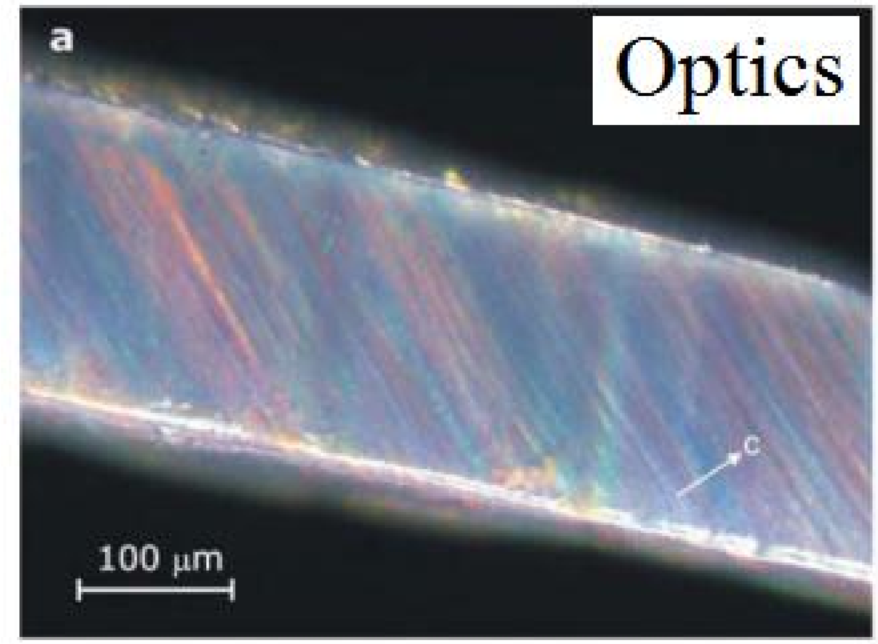
Рентгеновский микроскоп **реально** дает новые возможности

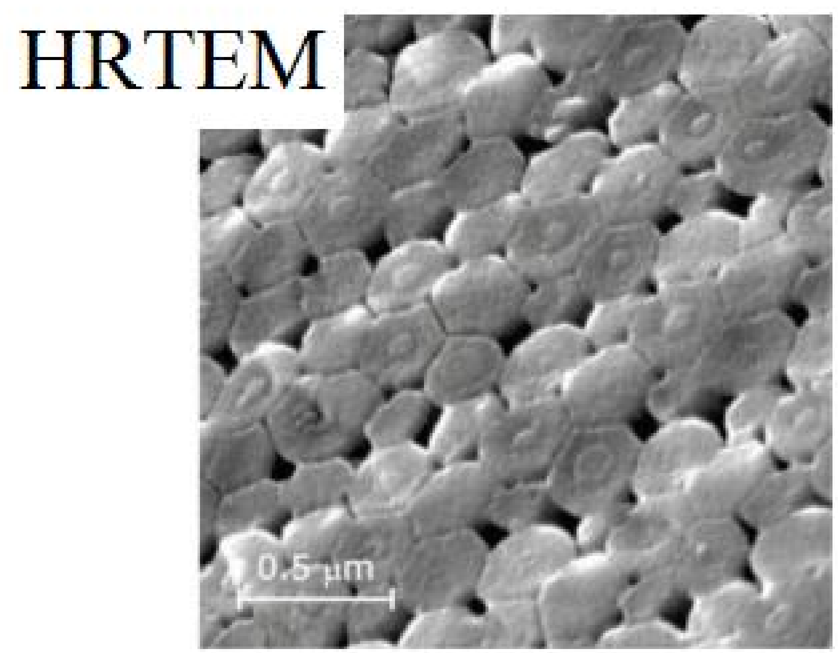
Это не игрушка, поиграли и бросили.

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*







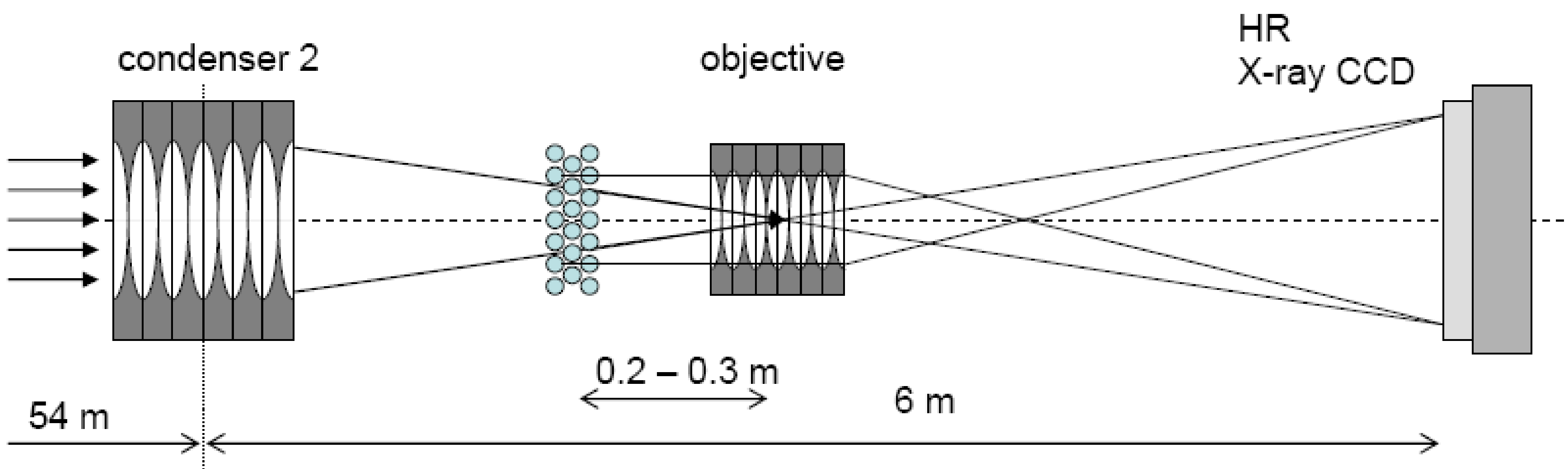
Adv. Mater. **2010**, 22, 3256–3259

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)

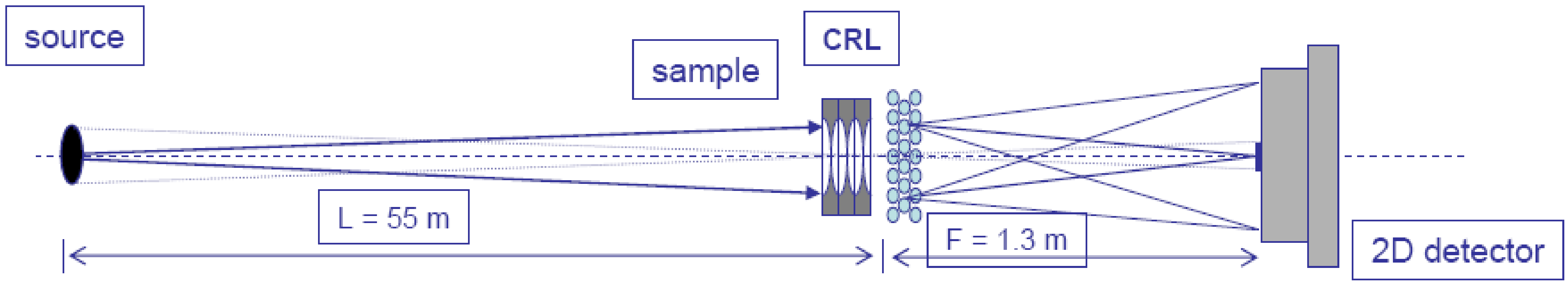
(2) – Objective CRL (objective) has a short focus length and it works as a microscop. Large magnification is necessary to adjust CCD detector resolution (about $1\ \mu m$)

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



Some CRL applications. Fourier images APL-2005-86-014102

X-ray High Resolution Diffraction Using Refractive Lenses



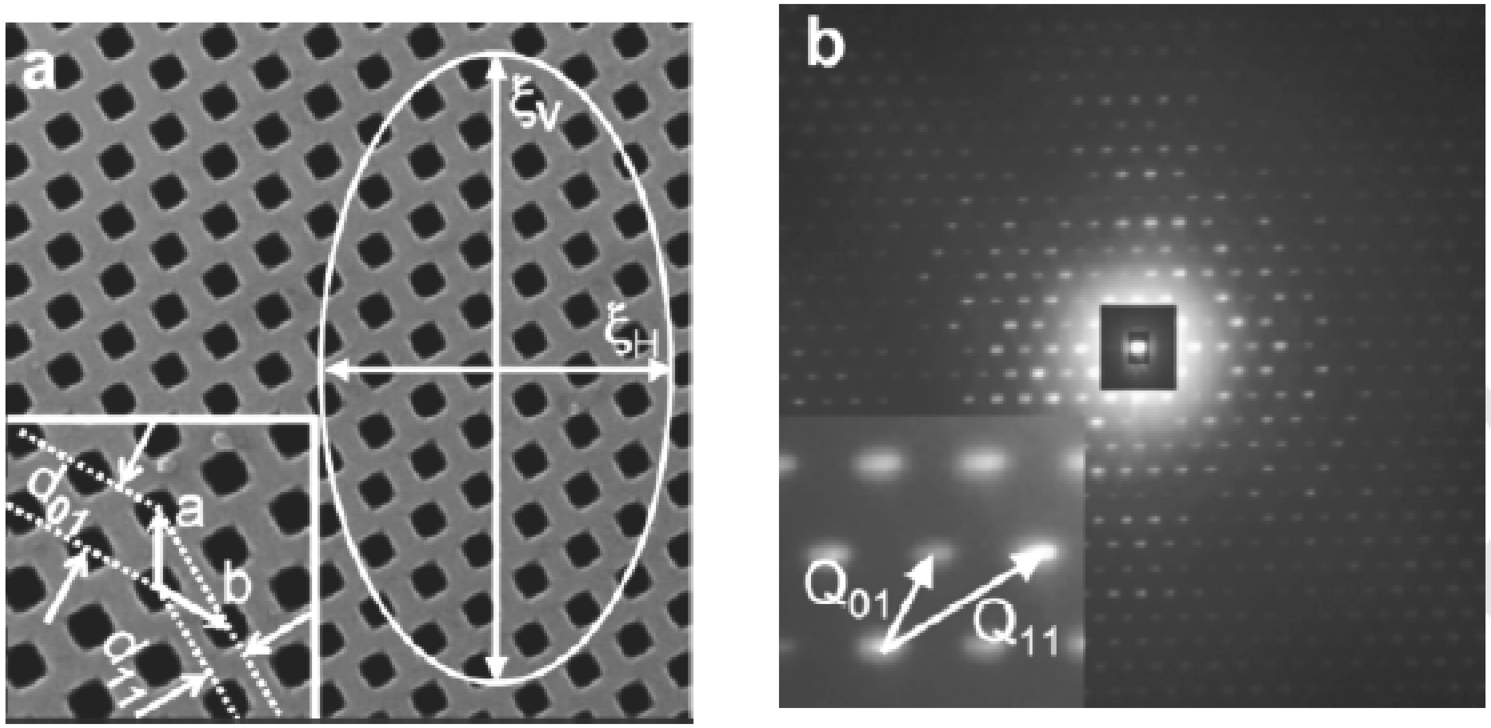
E = 28 keV
Al CRL, N = 112, F = 1.3 m

CCD resolution 2 μm
pixel / Θ = d

Resolution is limited
by angular source size:
s/L ~ 1 μrad

Momentum transfer
Resolution: 10^{-4} nm^{-1}

Si photonic crystal
a=b=4.2 μm d_{01}=3.6 μm d_{11}=2.1 μm



Lattice vectors $g_{01} = 1.75 \cdot 10^{-3}$ nm^{-1} $g_{11} = 3 \cdot 10^{-3}$ nm^{-1}

Theory allows one to account for an absorption in the CRL which influences high order peaks visibility Opt. Comm. 2003-216-247, JETP-2003-97-204

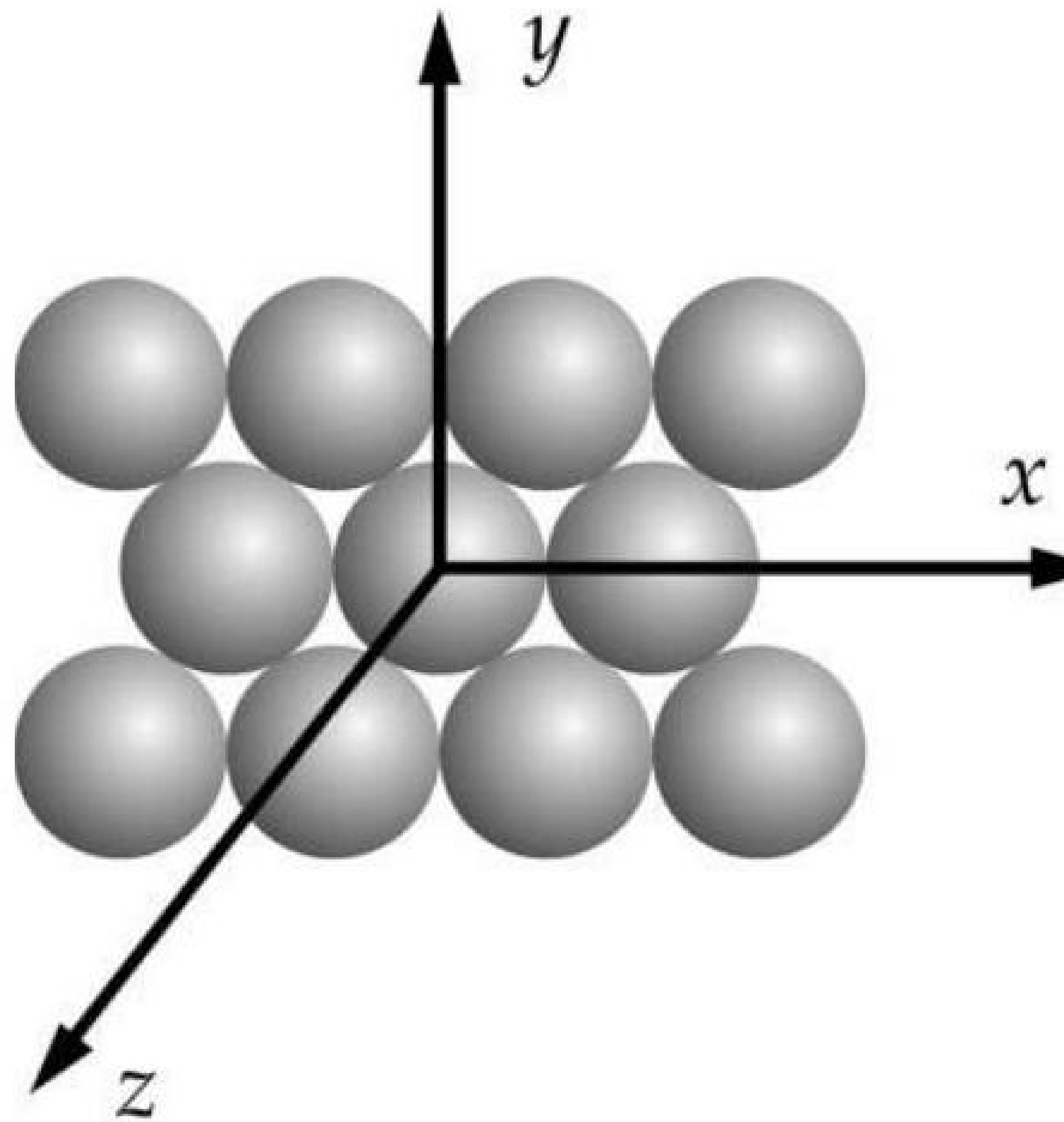


Figure 1
Coordinate axes relative to the photonic crystal.

$$E(\mathbf{r}, t) = \exp(ikz - i\omega t)\, A(\mathbf{r}, \omega),$$

$$\Box E(\mathbf{r}, t) = \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\int \mathrm{d}t'\, \chi(\mathbf{r}, t')E(\mathbf{r}, t - t'),$$

where

$$\Box = \Delta - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}, \qquad \Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

and $\chi(\mathbf{r}, t)$ is the time-dependent susceptibility of matter.

$$\frac{\partial A}{\partial z} = \frac{ik}{2}\chi(\mathbf{r}, \omega)A + \frac{i}{2k}\Delta A,$$

$$\frac{\partial A}{\partial z} = -ik\eta\rho(\mathbf{r})A + \frac{i}{2k}\left(\frac{\partial^2 A}{\partial x^2} + \frac{\partial^2 A}{\partial y^2}\right).$$

$$A = CB, \qquad C = \exp\left[-ik\eta \int_{z_0}^{z} \mathrm{d}z' \rho(x, y, z')\right].$$

$$\frac{\partial B}{\partial z} = \frac{i}{2k}\left[\frac{\partial^2 B}{\partial x^2} + \frac{\partial^2 B}{\partial y^2} + O(\mathbf{r})\right].$$

Here

$$O(\mathbf{r}) = C^{-1}\left[2\frac{\partial B}{\partial x}\frac{\partial C}{\partial x} + 2\frac{\partial B}{\partial y}\frac{\partial C}{\partial y} + B\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right)\right].$$

$$B(x, y, z) = \int \mathrm{d}x' \, \mathrm{d}y' P_2(\Delta x, \Delta y, \Delta z) B(x', y', z_0), \tag{9}$$

where $\Delta x = x - x'$, $\Delta y = y - y'$, $\Delta z = z - z_0$, $P_2(x, y, z) = P(x, z)P(y, z)$ and

$$P(x, z) = \frac{1}{(i\lambda z)^{1/2}} \exp\left(i\pi \frac{x^2}{\lambda z} \right) \tag{10}$$

is the Fresnel propagator.

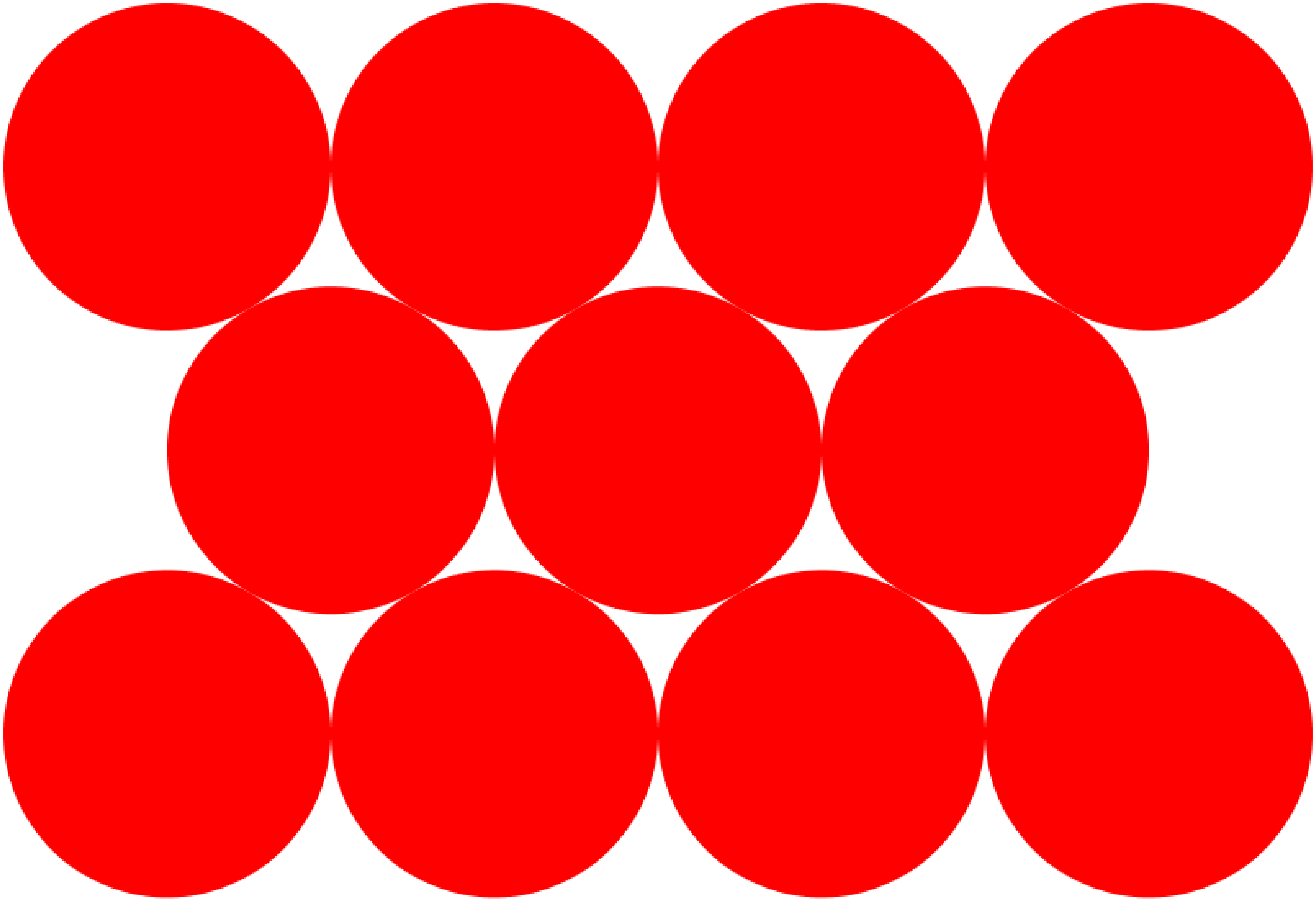
Finally, for the initial function we have the solution

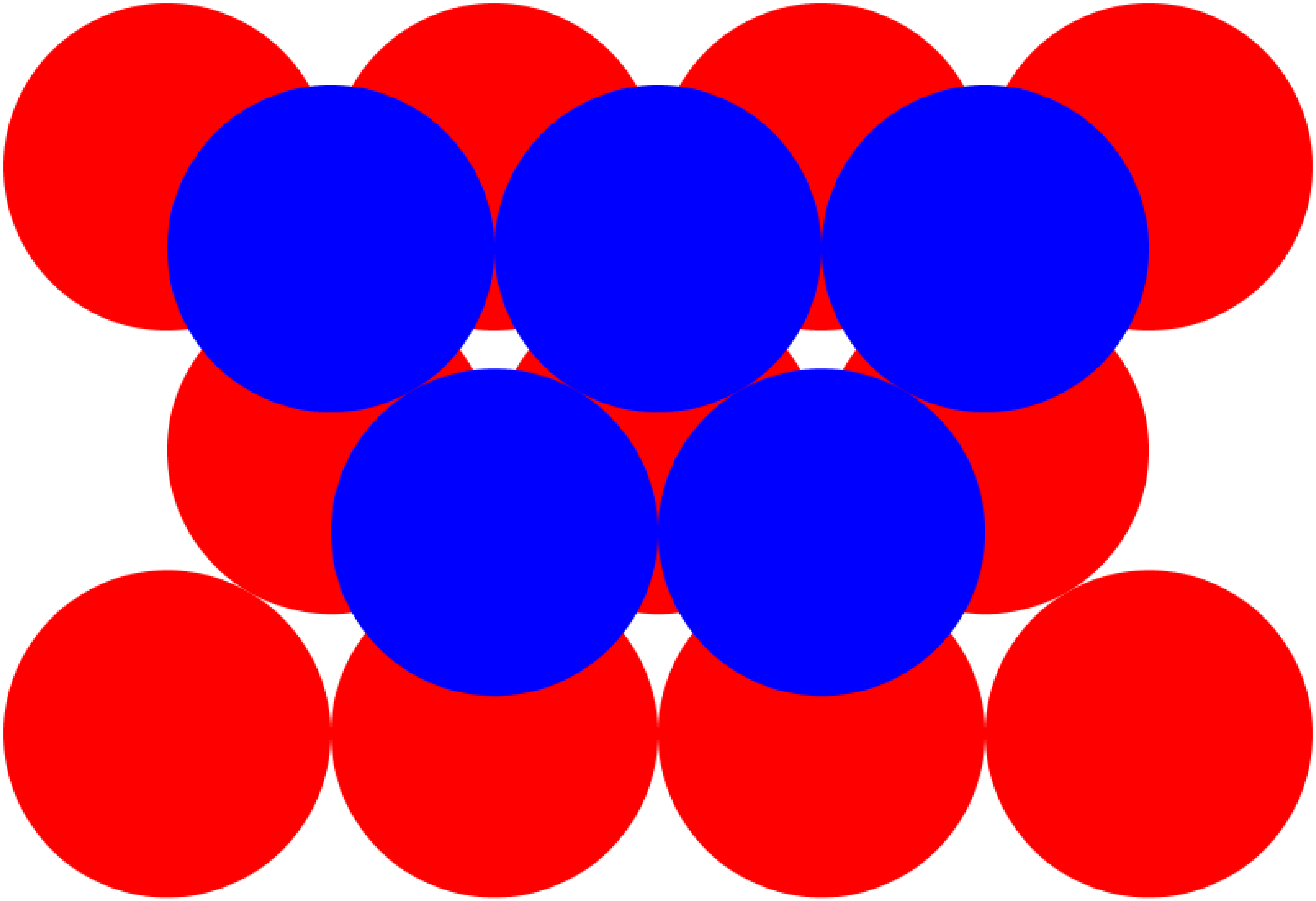
$$A(x, y, z) = \exp\left[-ik\eta \int_{z_0}^{z} \mathrm{d}z' \, \rho(x, y, z') \right] \times \int \mathrm{d}x' \mathrm{d}y' \, P_2(\Delta x, \Delta y, \Delta z) A(x', y', z_0). \tag{11}$$

$$A(z) = P_2(\Delta z/2) * C\,[P_2(\Delta z/2) * A(z_0)],$$

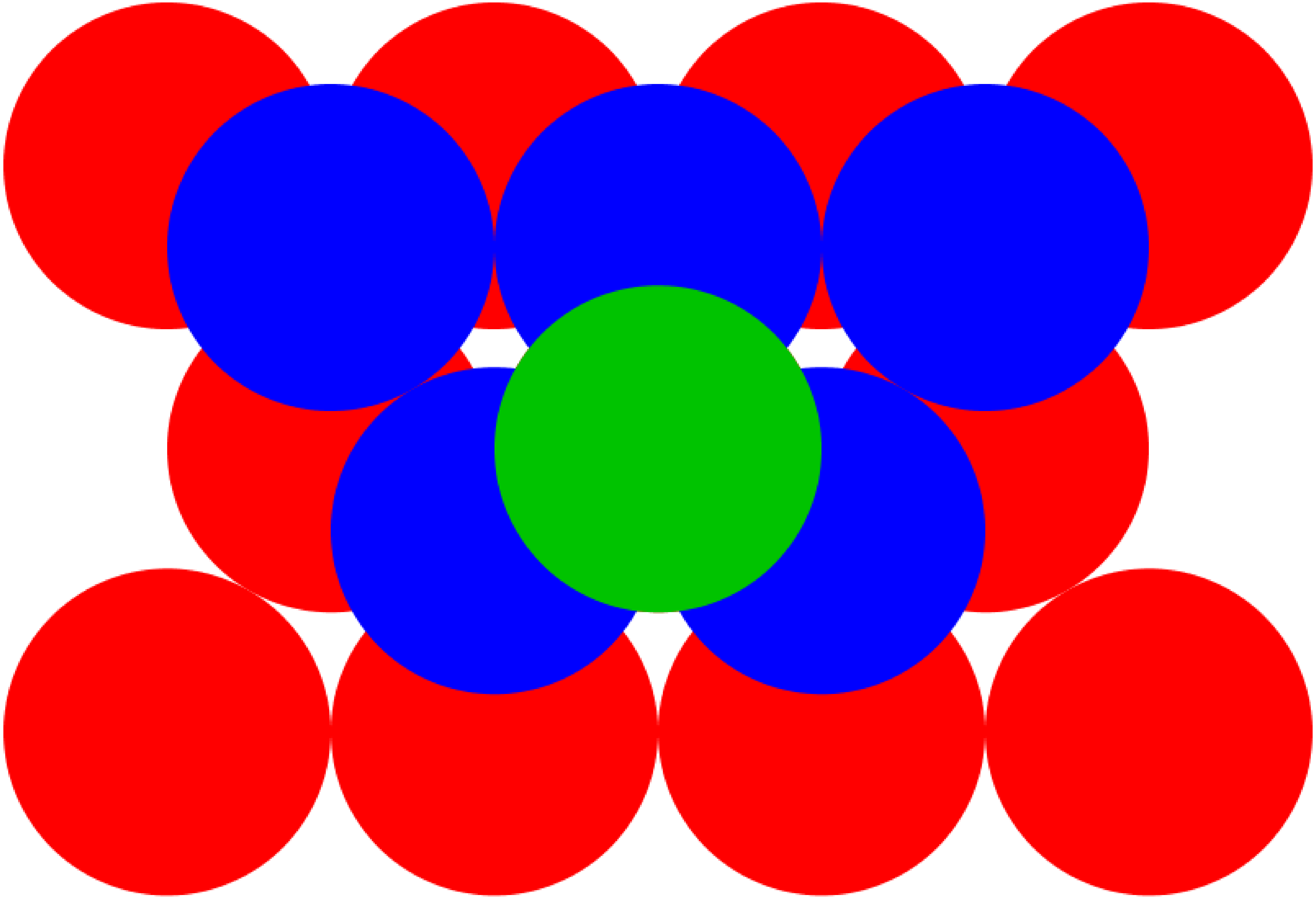
$$s(x, y) = \int_{z}^{z+h} \mathrm{d}z'\, \rho(x, y, z')$$

$$C(x, y) = \exp[-ik\eta\, s(x, y)].$$

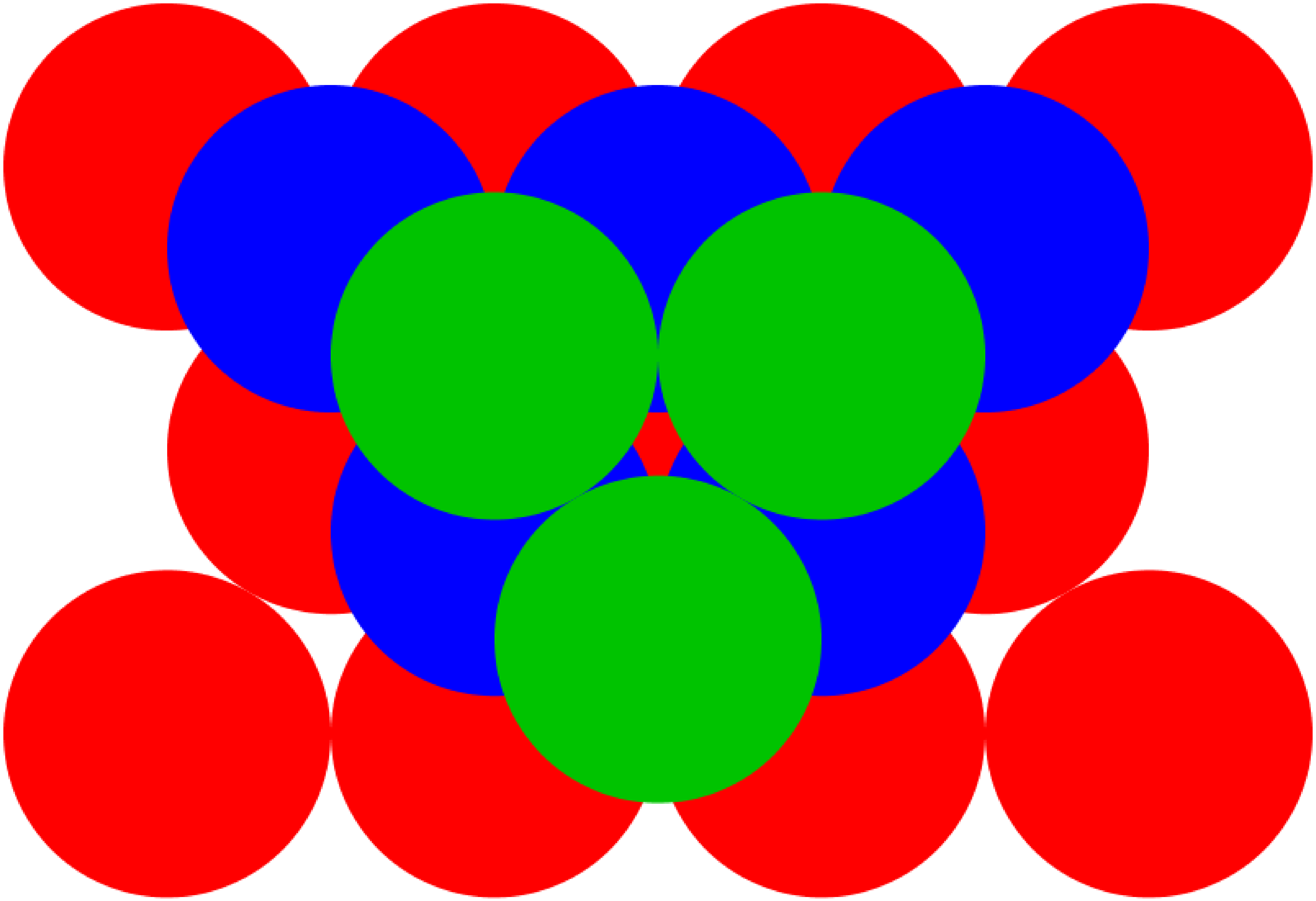




ГПУ решетка, имеет сквозные каналы



ГЦК решетка, 111 направление



Конкретный пример:
ГЦК решетка, инвертированный Ni кристалл, то есть никель заполняет пустоты, полистиреновые шарики удалены травлением в толуене за несколько часов
Период D = 0.5 мкм (500 нм), всего 9 слоев (3 периода)
Период вдоль оси Z равен $h = 3D(2/3)^{1/2}$ = 1.225 мкм
Расчет методом FFT на сетке 1024*1024 точек
Могу делать 4096*4096 и даже делал, но не надо.
Необходимо обрезать высокие частоты.
Первоначально вычислялось пропагирование по кристаллу
Затем по воздуху с шагом 4 мкм. **Больше нельзя** !
На каждой итерации убирались артефакты дифракции на щели из условия периодичности.

Function $s(x,y)$ as a linear black and white contrast

period along z axis is

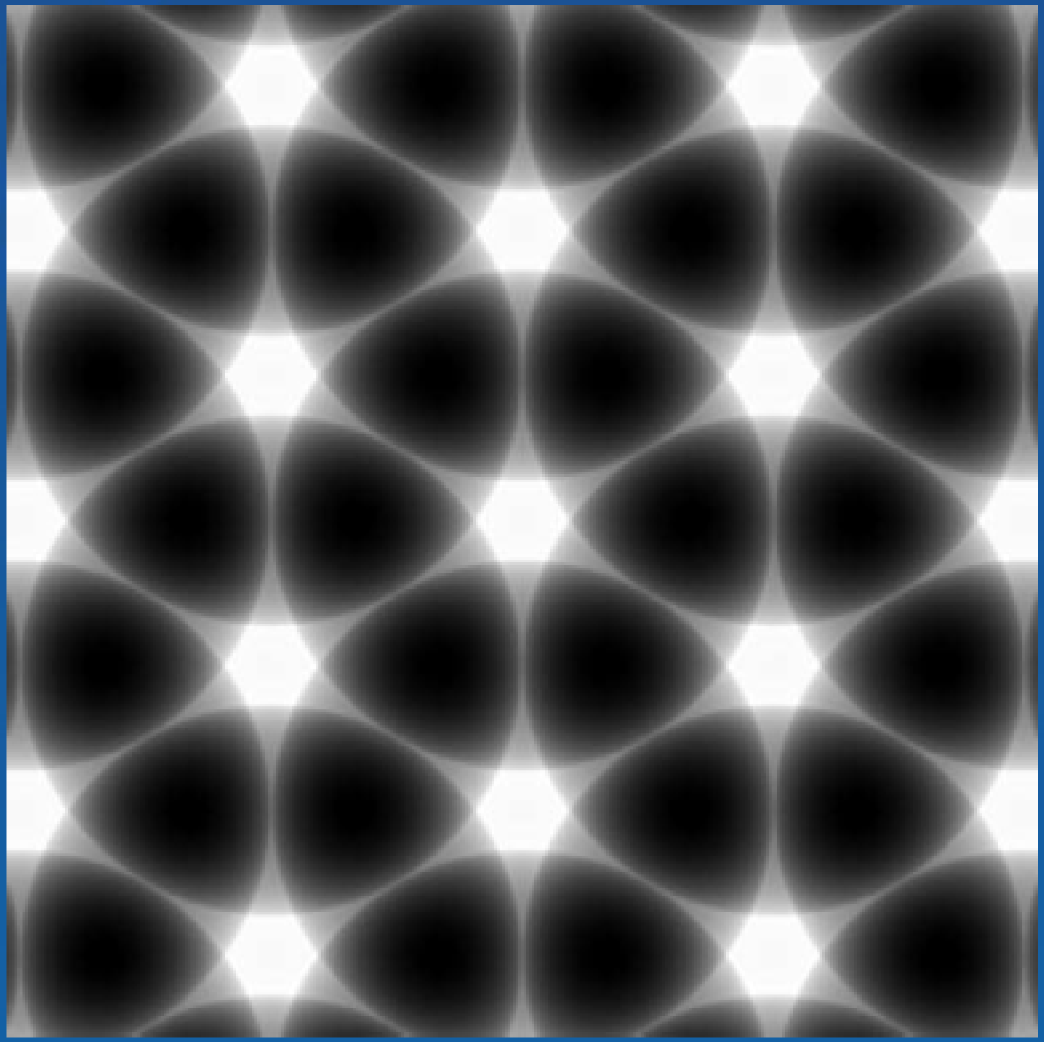
$$h = 3D\,(2/3)^{1/2} = 1.2247\ \mu m$$

the matter thickness for the period is described:

$$s(x,y) = \int_{z}^{z+h} d\,z' \rho(x,y,z')$$, where z is arbitrary

Simulation were performed on (x,y) plane

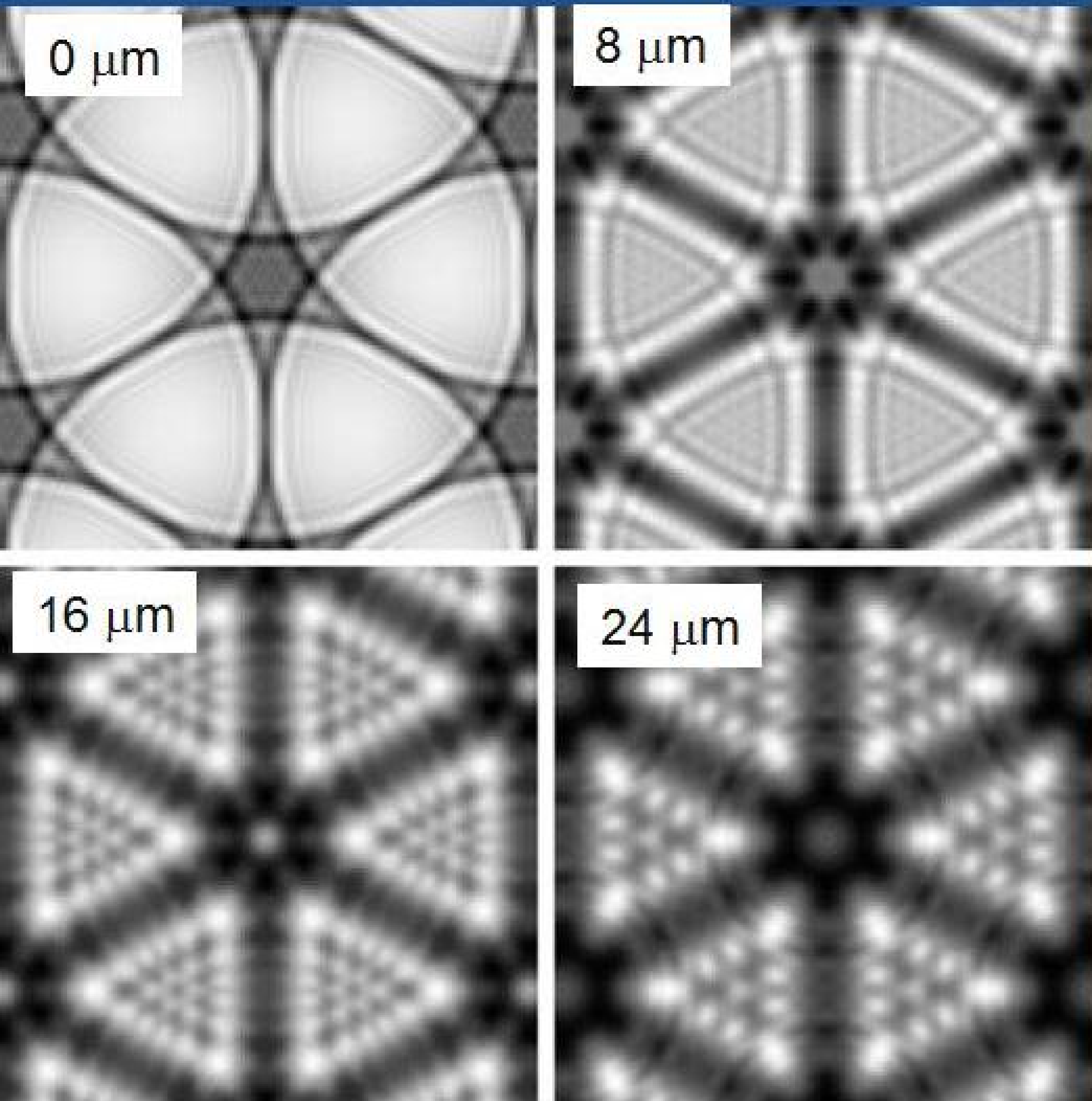
since function $s(x,y)$ is periodical
set of 1024x1024 points
with a step of 1nm was chosen



black color $s_{min} = 0.1067$
white color $s_{max} = 0.7331$

Periods are: 0.5 µm horizontally
0.2887 µm vertically

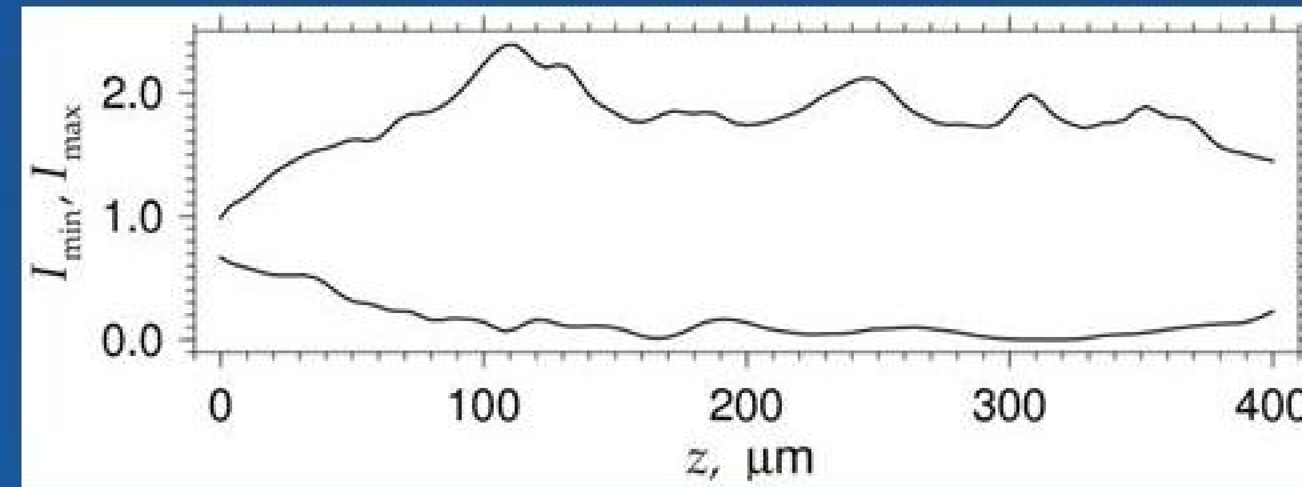
Intensity distribution of strongly modulated wave in free space behind the PhC



central area 512x512 points

1 period horizontally and longer region vertically to reveal the hexagonal symmetry of the image

Minimum and maximum values of relative intensity distributions at various distances.



Behind the photonic crystal the I_{min} is 0.67, while in front of the crystal it is 1.

The contrast at *z = 0* is low and is absorption.

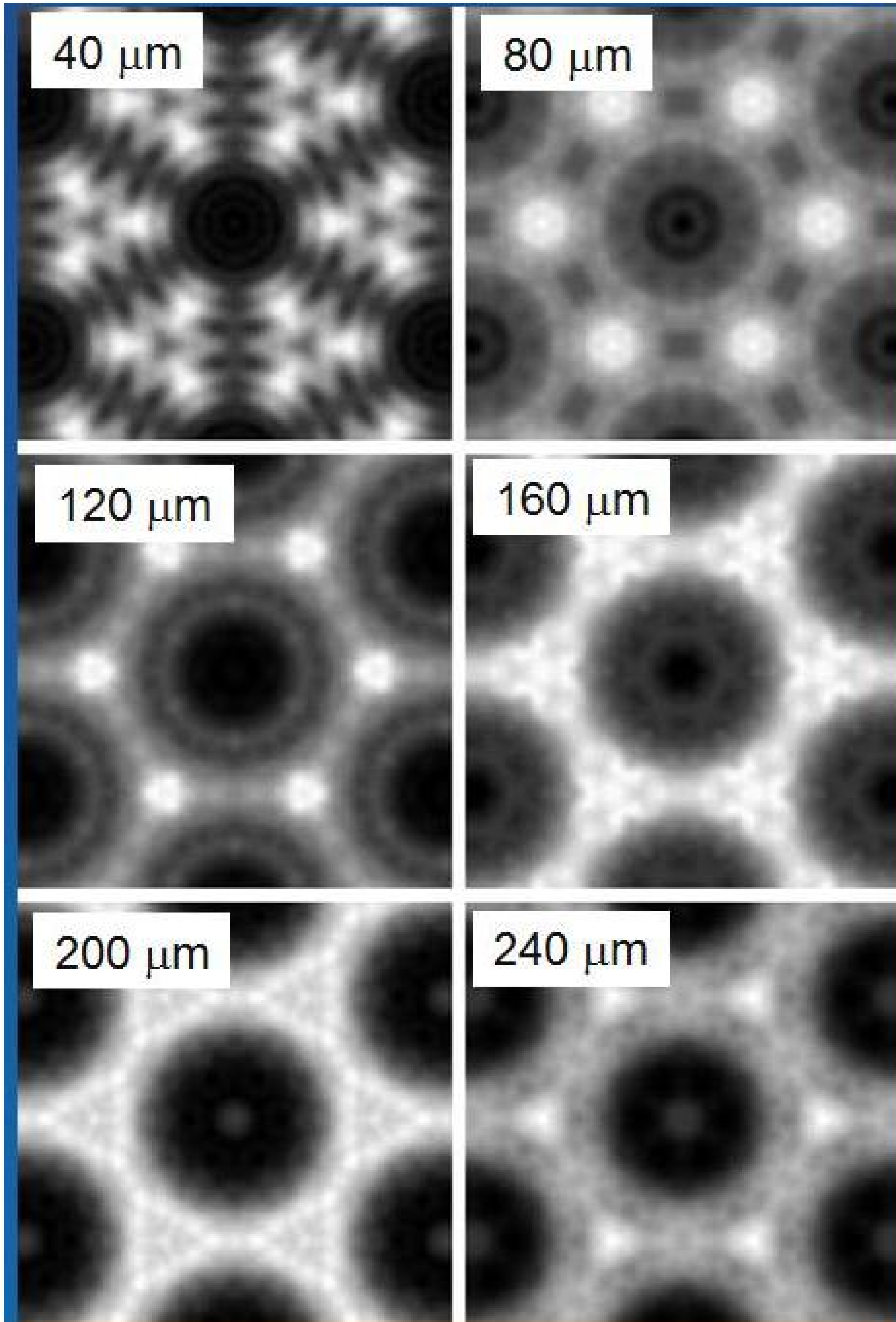
With increase z the phase contrast becomes more pronounced

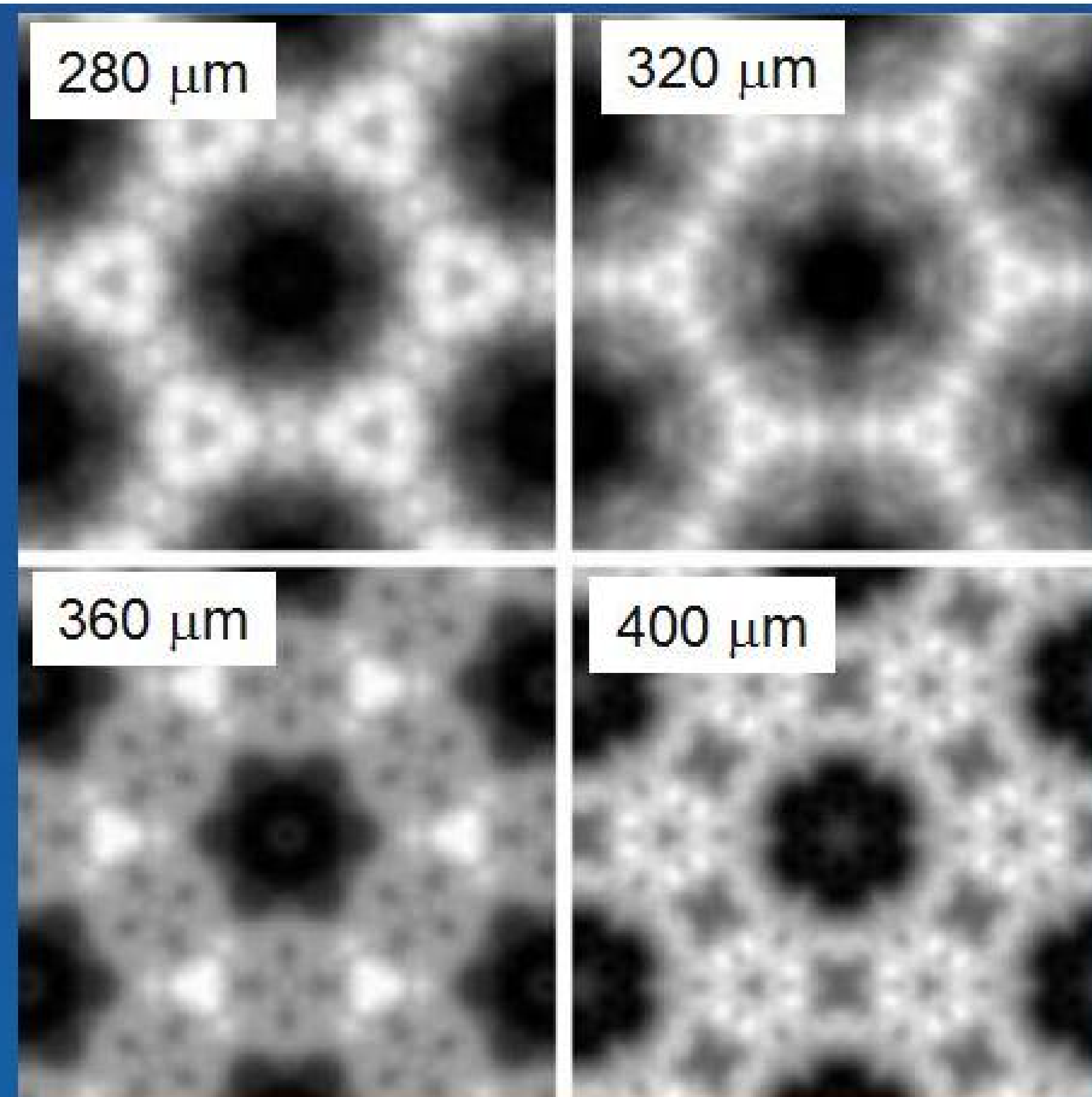
intensity distribution deviates more and more from the Ni thickness map

Interference fringes appear in the images

calculations were performed for the ideal situation:

- fully coherent radiation and
- unlimited detector resolution.





The content of the images changes significantly in each iteration step, but it is difficult to show 100 pictures.

However, they have some common features. The regions of minimum intensity always correspond to the regions of high Ni thickness.

Эффект Тальбо

Периодическое волновое поле с периодом p воспроизводит себя на расстоянии Тальбо $z_T = 2p^2/\lambda$. В нашем случае λ = 0.1 нм минимальный период p = 0.289 мкм (по вертикали).

Вычисляя, получаем z_T = 1667 мкм. Это в 4 раза больше !

$$A(x,0) = \sum_{m=-\infty}^{\infty} A_m \exp(i2\pi mx/p).$$

Then the convolution

$$A(x,z) = \int \mathrm{d}x' \, P(x-x',z)\, A(x,0)$$

has an analytical solution.

The result can be written as follows,

$$A(x,z) = \sum_{m=-\infty}^{\infty} A_m \exp(i2\pi mx/p - i\pi m^2 \lambda z/p^2)$$

БЛАГОДАРЮ

ЗА

ВНИМАНИЕ