Supplemental material to the article
"Evolution of scattering patterns for dielectric metasurfaces"

We define the structure factor as a sum [1]:

$$S(\mathbf{q}) = \sum_j \exp(i\mathbf{r}_j\mathbf{q}), \tag{1}$$

where $\mathbf{q} = \mathbf{k}_i - \mathbf{k}_s$ is the scattering vector, $\mathbf{k}_i$ and $\mathbf{k}_s$ are the incident and scattering wave vectors, and r_j is a scatterer position. In many systems scattering intensity can be evaluated by $|S(\mathbf{q})|^2$. Below we analyze several types of scatterer distributions and calculate their structure factors.

1. Linear chain

We start from the simplest structure that is a chain of N scatterers laying along an axis $\mathbf{a}$ hexagon. The scatterer position is defined by $r_j = n\mathbf{a}$, where n is non-negative integer less than N. The sum in (1) can be evaluated as [1]

$$\sum_{n=0}^{N-1} \exp(\mathrm{i}nx) = \frac{\sin(Nx/2)}{\sin(x/2)} \exp(\mathrm{i}(N-1)x/2). \tag{2}$$

The scattering pattern of the chain is represented by a number of cones being coaxial with $\mathbf{a}$. For the case of normal incidence one of the cones degenerates into a plane.

2. Parallelogram structure

Let the scatterers positions are defined by $r_j = n_1\mathbf{a}_1 + n_2\mathbf{a}_2$, where $\mathbf{a}_1$ and $\mathbf{a}_2$ are lattice vectors, and n_1 and n_2 are non-negative integers less than N_1 and N_2. The scatterers are bounded by a parallelogram and taking into account (2) the scattering factor can expressed as

$$S(\mathbf{q}) = \frac{\sin(N_1\mathbf{q}\mathbf{a}_1/2)}{\sin(\mathbf{q}\mathbf{a}_1/2)} \frac{\sin(N_2\mathbf{q}\mathbf{a}_2/2)}{\sin(\mathbf{q}\mathbf{a}_2/2)} \exp\left(i\mathbf{q}\frac{(N_1-1)\mathbf{a}_1 + (N_2-1)\mathbf{a}_2}{2}\right). \tag{3}$$

The scattering pattern is obtained by a product of two scattering factors for chains along $\mathbf{a}_1$ and $\mathbf{a}_2$. The direction at which the cones intersect each other a strong scattering maximum to appear.

3. Hexagonal structure

Now we consider the scatters arranged in the hexagonal lattice and bounded by a hexagon. If N is even number we splits the hexagons into 3 parallelograms and evaluate $S(\mathbf{q})$ as a sum of three parallelogram structure factors (3) as

$$S(\mathbf{q}) = S_{12}(\mathbf{q}) \exp\left(\frac{\mathrm{i}\mathbf{q}\mathbf{a}_1}{2}\right) + S_{23}(\mathbf{q}) \exp\left(-\frac{\mathrm{i}\mathbf{q}\mathbf{a}_1}{2}\right) + S_{31}(\mathbf{q}) \exp\left(\frac{\mathrm{i}\mathbf{q}(\mathbf{a}_3 - \mathbf{a}_2)}{2}\right). \tag{4}$$

Next we analyze the scattering pattern along vertical plane. We assume the sample is illuminated normally $\mathbf{k}_i = (0, 0, k)$ and the scattering wave vector is $\mathbf{k}_s = (0, k\sin\varphi, k\cos\varphi)$. By introducing $\zeta = (k\sqrt{3}a\sin\varphi)/4$ the scattering factor for the hexagonal samples in the vertical plane is approximated by

$$|S(\mathbf{q})|^2 \approx N^2 \frac{\sin^2(2N\zeta)}{\sin^2(\zeta)}. \tag{5}$$

4. Graphene-type structure

In this section we discuss scattering from graphene-type samples. To evaluate the structure factor we summarize six parallelogram' structure factors (3)

$$S(\mathbf{q}) = S_{12}(\mathbf{q}) \left\{e^{i\mathbf{q}\frac{\mathbf{a}_1-\mathbf{a}_3}{3}} + e^{i\mathbf{q}\frac{\mathbf{a}_2-\mathbf{a}_3}{3}}\right\} + S_{23}(\mathbf{q}) \left\{e^{i\mathbf{q}\frac{\mathbf{a}_2-\mathbf{a}_1}{3}} + e^{i\mathbf{q}\frac{\mathbf{a}_3-\mathbf{a}_1}{3}}\right\} + S_{31}(\mathbf{q}) \left\{e^{i\mathbf{q}\frac{\mathbf{a}_3-\mathbf{a}_2}{3}} + e^{i\mathbf{q}\frac{\mathbf{a}_1-\mathbf{a}_2}{3}}\right\}. \tag{6}$$

Now we evaluate the structure factor for scattering into the vertical plane, which read

$$S(\mathbf{q}) = N\frac{\sin(N\zeta)}{\sin(\zeta)} e^{-\mathrm{i}(N-1)\zeta} \left\{e^{-\frac{2i\zeta}{3}} + e^{-\frac{4i\zeta}{3}}\right\} + \frac{\sin^2(N\zeta)}{\sin^2(\zeta)} \left\{e^{-\frac{2i\zeta}{3}} + e^{\frac{2i\zeta}{3}}\right\} + N\frac{\sin(N\zeta)}{\sin(\zeta)} e^{\mathrm{i}(N-1)\zeta} \left\{e^{\frac{4i\zeta}{3}} + e^{\frac{2i\zeta}{3}}\right\}. \tag{7}$$

After simplification this formula has a form

$$S(\mathbf{q}) = \frac{\sin(N\zeta)}{\sin(\zeta)} \left(4N \cos(N\zeta) \cos\left(\frac{\zeta}{3}\right) + 2\frac{\sin(N\zeta)}{\sin(\zeta)} \cos\left(\frac{2\zeta}{3}\right) \right). \tag{8}$$

The second term of sum is negligible, hence the resulting formula for the structure factor read

$$S(\mathbf{q}) \approx 2N \frac{\sin(2N\zeta)}{\sin(\zeta)} \cos(\zeta/3). \tag{9}$$

This expression resembles one for the hexagonal samples (5) but it has an additional factor $\cos(\zeta/3)$, which is responsible to the gap formation in the arcs being observed in the graphene diffraction patterns.

References

[1] A. Guinier. *X-Ray Diffraction. In Crystals, Imperfect Crystals, and Amorphous Bodies*, W.H. Freeman and Co, San Francisco and London (1963).