# Photonic density of states calculation (plane wave method)

- Definition of the conventional unit cell
  - bravais lattice
  - length of sides: $a, b, c$
  - angles: $\alpha, \beta, \gamma$
  - $\epsilon_C$ of unit cell
  - position, radius and $\epsilon_S$ of spheres
- Construction of simple unit cell (3D matrix $C$ with the right $\epsilon$-values)
- Construction of the reciprocal unit cell (first brillouin zone)
- Calculation of the fourier coefficients $f = fft3(C)$ and selection of a certain number of fourier coefficients $f_{sel}$ within a finite sphere in reciprocal space
- Graphical presentation of the selected fourier coefficients $f_{sel}$ and the primitive unit cell in reciprocal space
- Inverse fourier transformation of the selected fourier coefficients $C' = ifft3(f_{sel})$ for a graphical density map of the primitive unit cell in real space (to check the real $\epsilon$-distribution used for further calculations)
- Construction of the matrix\(^1\) (hermitian), whose eigen values are the $c^2\omega^2$
- Calculation of the eigen values for equal spaced points in several specified directions in the reciprocal unit cell (dispersion relation), graphical presentation
- Calculation of the eigen values for a discrete subdivision of the reciprocal unit cell and counting the occurring frequencies (density of states; $D(\omega)$), graphical presentation and .txt-file for further use

\(^1\)Photonic band structure calculations for 2D and 3D photonic crystals; Chapter 2.3: Plane Wave Expansion of Maxwell's Equations; Aaron Vincent Morton; 2002
2 simple cubic

- Conventional unit cell: $a = 100\,nm; \epsilon_C = 1$
- One close packed sphere with $\epsilon_S = 13$

Figure 1: Primitive unit cell in real space and reciprocal space

Figure 2: Dispersion relation and density of states
3 inverse face centered cubic

- Conventional unit cell: $a = 100\, \text{nm}$; $\epsilon_C = 13$
- One close packed sphere with $\epsilon_S = 1$

Figure 3: Primitive unit cell in real space and reciprocal space

Figure 4: Dispersion relation and density of states
4 diamond structure

- Conventional unit cell: $a = 100\, nm; \epsilon_C = 1$
- Two close packed spheres with $\epsilon_S = 13$

![Diamond Structure Diagram](image)

Figure 5: Primitive unit cell in real space and reciprocal space

![Dispersion Relation and Density of States](image)

Figure 6: Dispersion relation and density of states
5 inverse diamond structure

- Conventional unit cell: $a = 100 \text{ nm}; \epsilon_C = 13$
- Two close packed spheres with $\epsilon_S = 1$

Figure 7: Primitive unit cell in real space and reciprocal space

Figure 8: Dispersion relation and density of states
6 hexagonal crystal structure

- Conventional unit cell: $a = b = c = 100 \text{nm}; \alpha = \beta = 90^\circ \text{deg}; \gamma = 120^\circ \text{deg}; \epsilon_C = 1$
- One sphere with $\epsilon_S = 13$; radius = $50 \text{nm}$

Figure 9: Primitive unit cell in real space and reciprocal space

Figure 10: Dispersion relation and density of states