Photonic crystal calculations

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1 Photonic density of states claculation (plane wave method)

- Definition of the conventional unit cell
  - bravais lattice
  - length of sides: a, b, c
  - angles: α, β, γ
  - ϵ_C of unit cell
  - position, radius and ϵ_S of spheres
- Construction of simple unit cell (3D matrix C with the right ϵ-values)
- Construction of the reciprocal unit cell (first brillouin zone)
- Calculation of the fourier coefficionts $f = fft3(C)$ 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 ϵ-distribution used for further calculations)
- Construction of the matrix[1] (hermitian), who's 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 occuring 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 $\epsilon_S = 13$

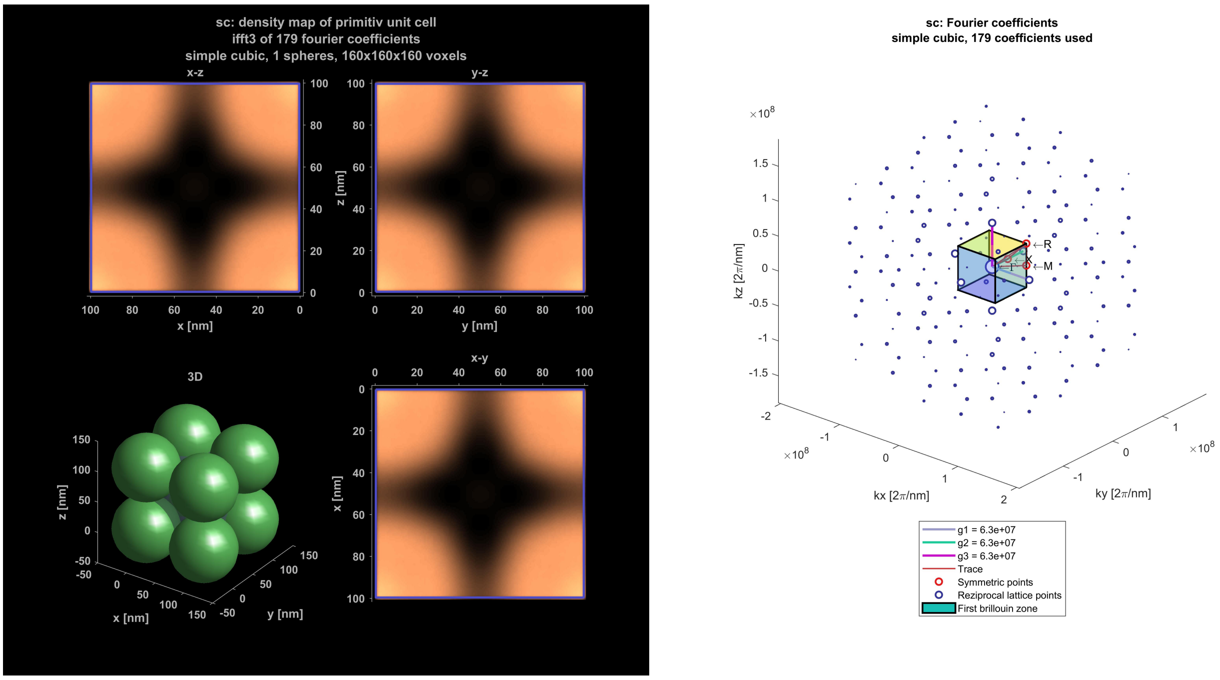


Figure 1: Primitive unit cell in real space and reciprocal space

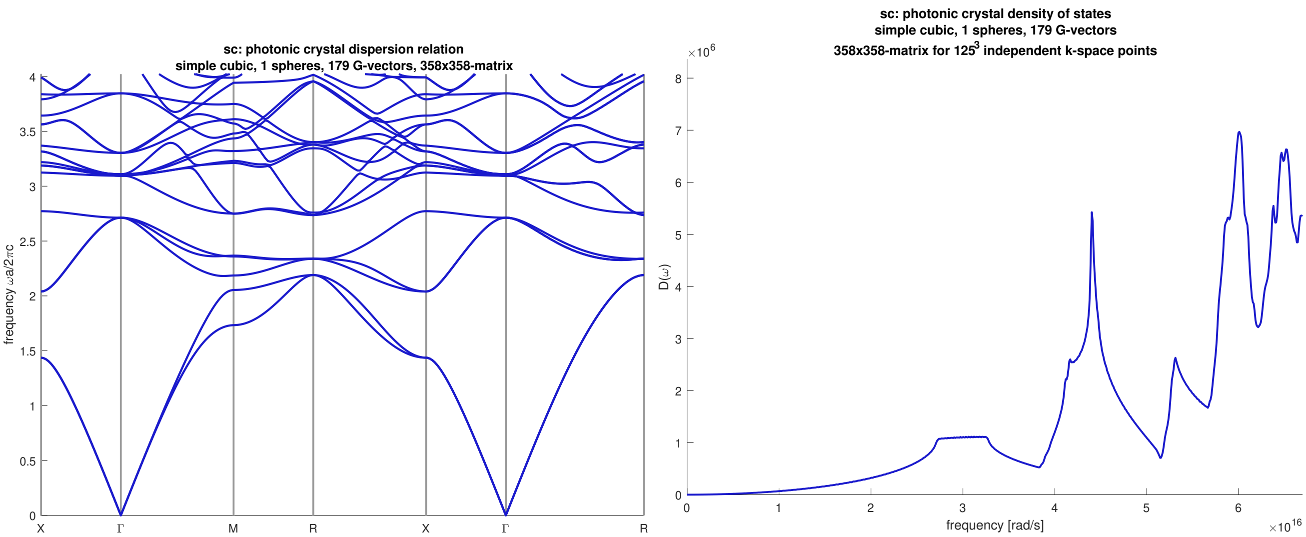


Figure 2: Dispersion relation and density of states

3 inverse face centered cubic

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

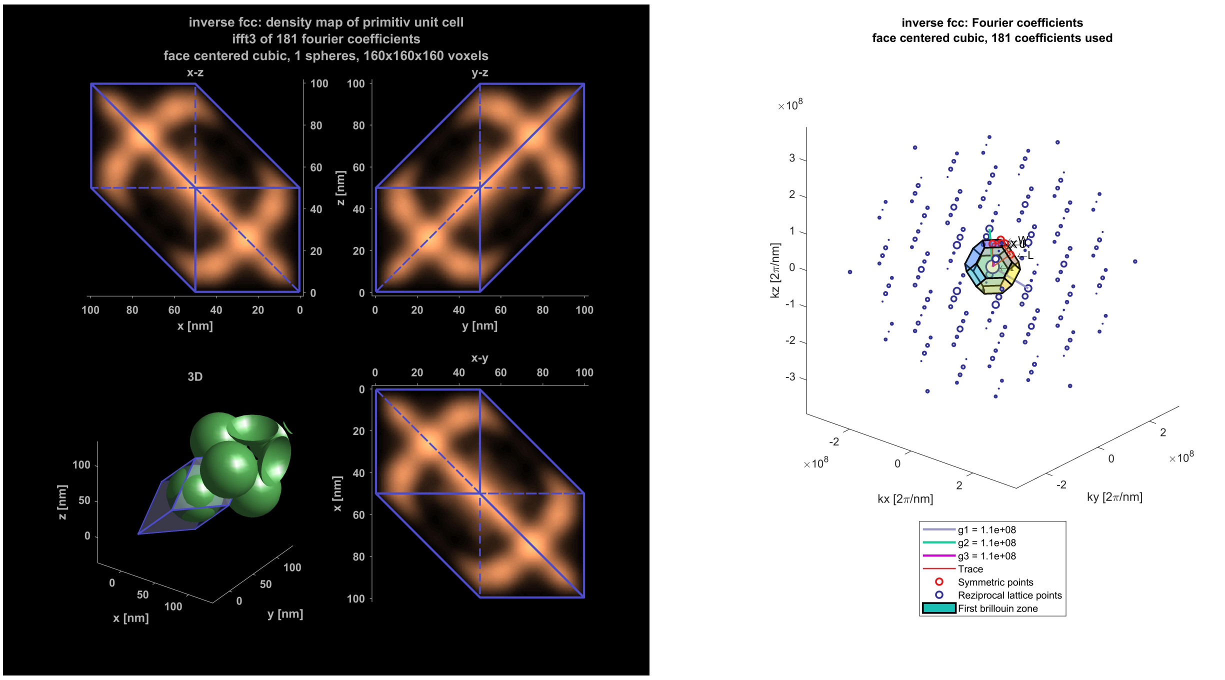


Figure 3: Primitive unit cell in real space and reciprocal space

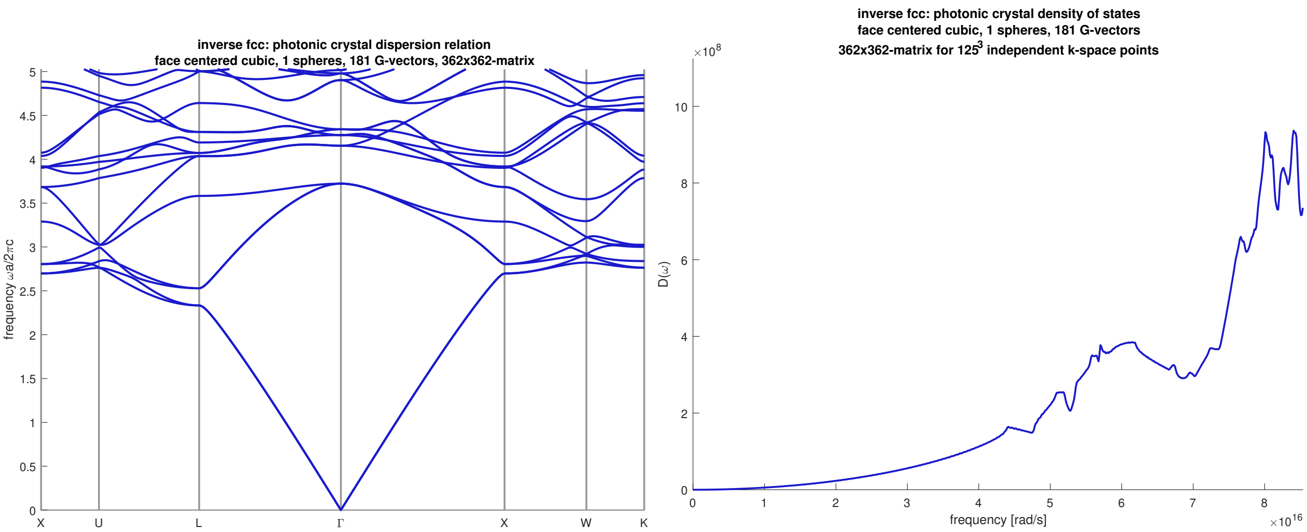
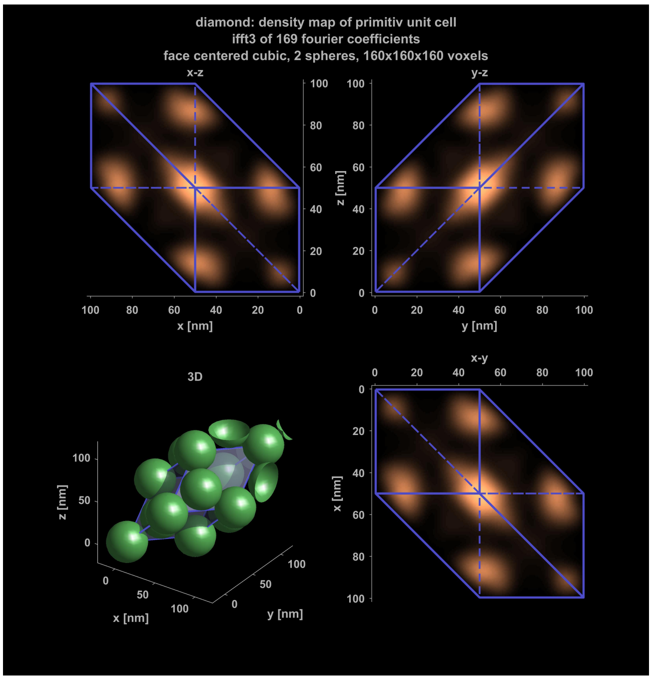


Figure 4: Dispersion relation and density of states

4 diamond structure

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



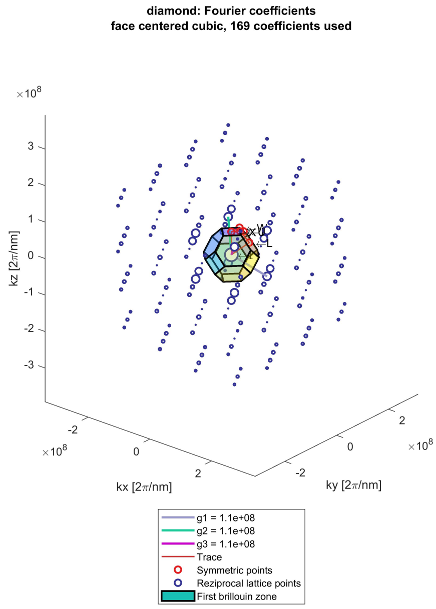
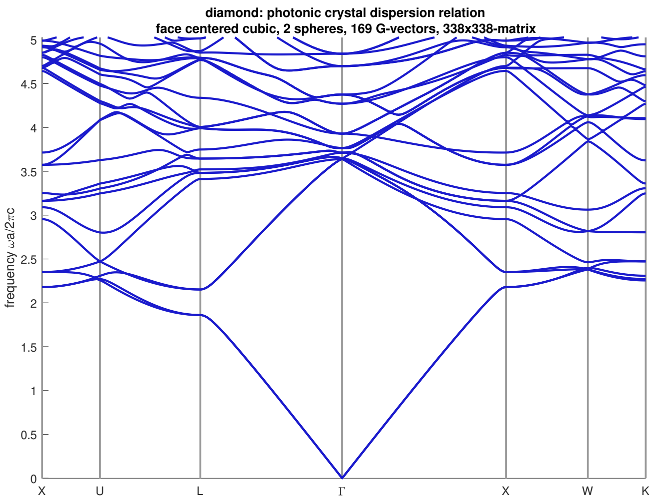


Figure 5: Primitive unit cell in real space and reciprocal space



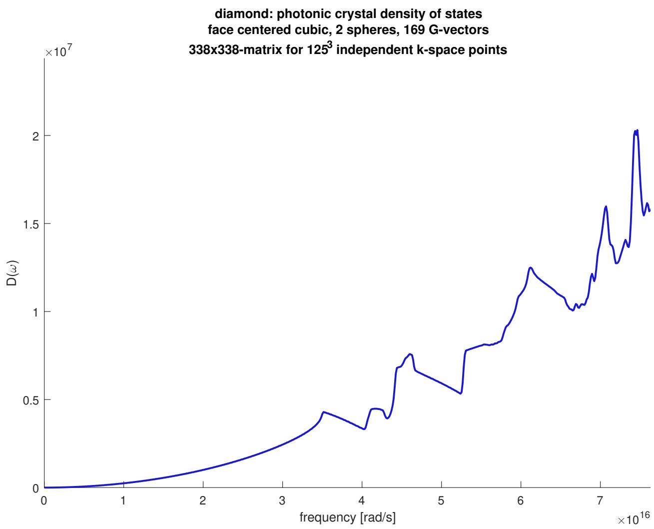


Figure 6: Dispersion relation and density of states

5 inverse diamond structure

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

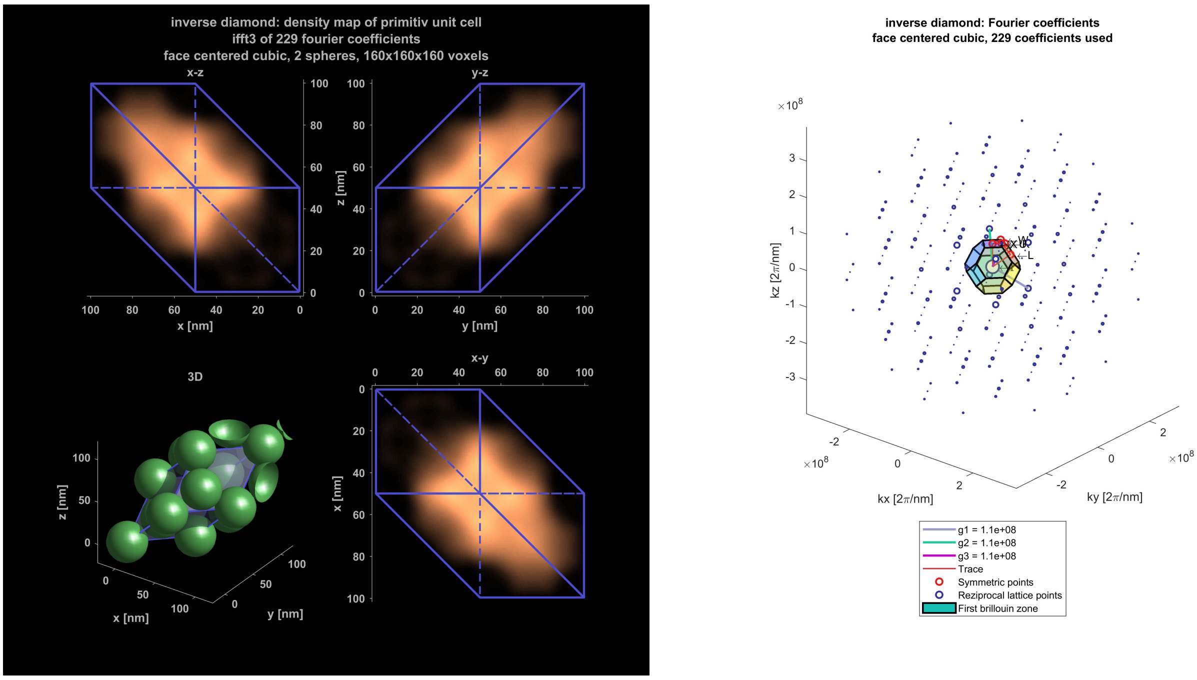


Figure 7: Primitive unit cell in real space and reciprocal space

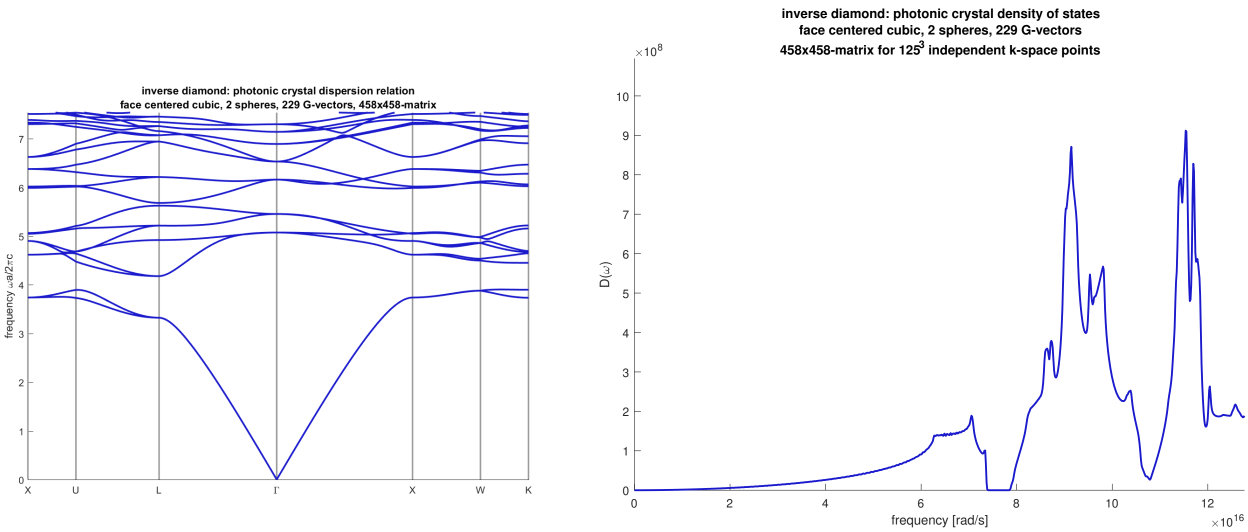
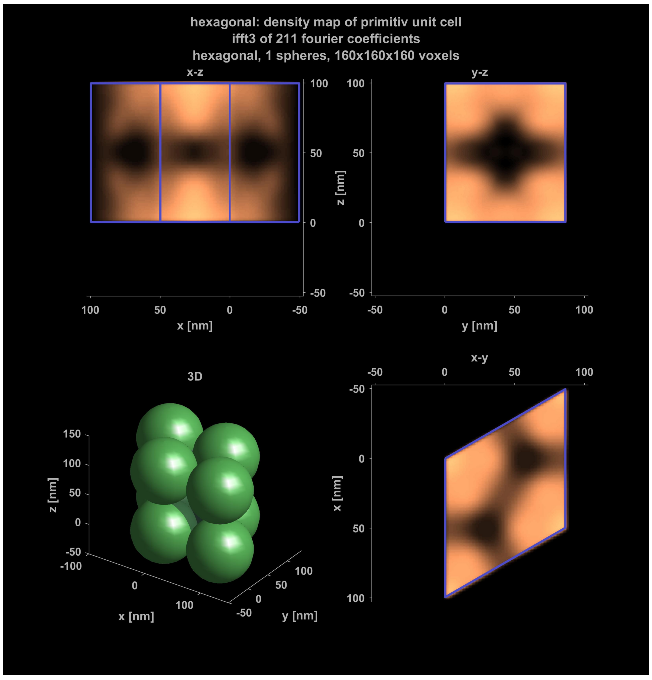


Figure 8: Dispersion relation and density of states

6 hexagonal crystal structure

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



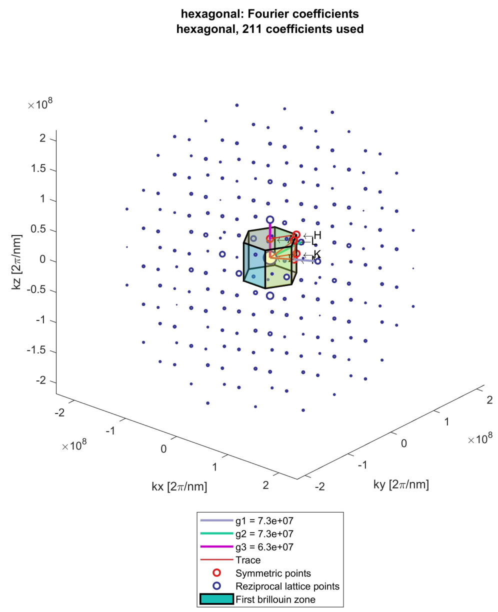
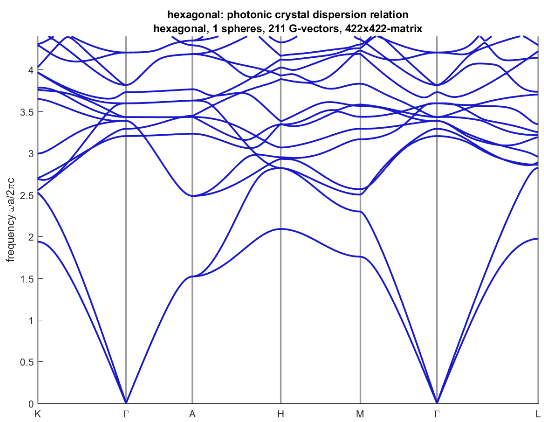


Figure 9: Primitive unit cell in real space and reciprocal space



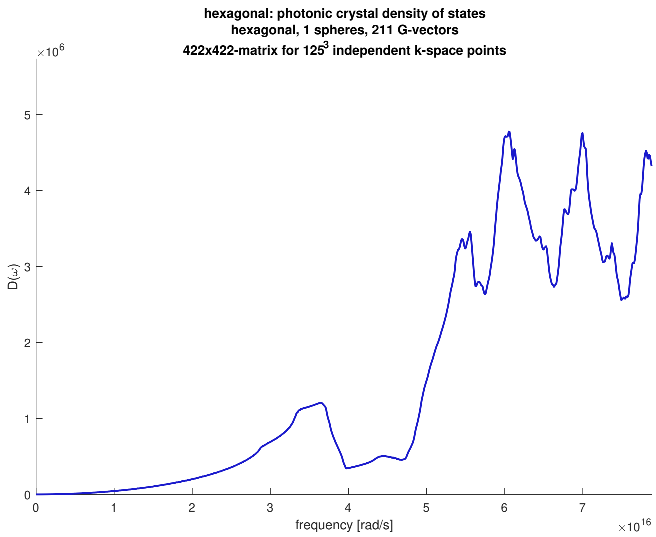


Figure 10: Dispersion relation and density of states