Surface electric potential of linear periodic charge density

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Abstract. Distribution of the surface electric potential allows visualizing surface plasmons and gives information about parameters of the plasmons. Some plasmonic structures have a periodic structure, for example hybrid self-assembled photonic-plasmonic crystals. Earlier we presented a new method of calculation of the potential for quasiperiodic and periodic structures. In this paper we compare the method with other methods that have different algorithms and formulas.

1. Introduction

Photonic-plasmonic crystals (PPCs) [1–7] have attracted increased attention recently. PPC is a hybrid structure with combination of dielectric nanophotonic elements with metallic ones supporting surface plasmon polaritons (SPP) [5]. Photonic crystals are materials with spatial periodicity in their dielectric function (or, equivalently, a periodical index of refraction) [8]. Such periodicity yields a strong modification of the electromagnetic field that manifests itself in new quantum electrodynamical effects [9]. PPC are used for easily coupled whispering gallery plasmons [10], surface-enhanced Raman spectroscopy [11, 12], coherent fluorescence emission [13], etc. The effect of surface plasmon resonance underlies the unusual properties of PPC. SPP are electromagnetic excitations propagating at the interface between a dielectric and a conductor [14]. Surface plasmons are collective oscillations in electron density at the surface of a metal [15]. The plasmons influence the surface electric potential. The potential gives rich information about properties and characteristics of the plasmons. Kelvin Probe Force Microscopy (KPFM) allows to use this advantage. It’s a modification of atomic force microscopy, which allows to obtain a map of potential distribution [16]. KPFM is an exceptional method for imaging and characterization of plasmonic modes at optical frequencies [17]. Findings [17] opened the way for using KPFM under optical illumination for direct imaging of SPPs with nanometric spatial resolution and sensitivity, established KPFM as a preferred candidate for experimental characterization of SPP nanodevices.

Using KPFM can give advantages to investigation of PPC. Because of dealing with a periodically structured medium, we can use advantages and methods, which are developed for periodic medium, the Bloch’s theorem [18] for example. By applying the theorem to distributions of charge and potential a new method of building the map of electric potential distribution was developed [19]. In this work, we used the method for calculation the map of electric potential...
distribution for an infinitely long, thin periodically charged thread and compared the method with other methods, that have different algorithms and formulas.

2. Results

We take an infinitely long, thin periodically charged thread as an object for comparison of methods for calculation of distribution of the electric potential. The potential can be determined via the Coulomb’s law:

\[ V(\mathbf{r}) = \int \frac{\rho(\mathbf{r}')}{4\pi\varepsilon_0 |\mathbf{r} - \mathbf{r}'|} d^3\mathbf{r}' , \tag{1} \]

where \( V \) is the potential, \( \rho \) is the volume charge density.

Let us write the charge distribution for our object:

\[ \rho(x, y, z) = \lambda_0 \cos(x) , \tag{2} \]

where \( \lambda_0 \) is the linear charge density.

Substituting (2) into (1), we obtain:

\[ V(x, y, z) = \frac{1}{4\pi\varepsilon_0} \lambda_0 \int \frac{\cos(x)}{\sqrt{(x - x')^2 + (y - y')^2}} dx dy . \tag{3} \]

The calculation of the electric potential, obtained by expression (3) for the infinitely long, thin periodically charged thread, lying along the axis x is presented in figure 1. We used the trapezoidal rule for calculation of the integral.

\[ \text{Figure 1. Distribution of the electric potential for } \lambda_0 = 10^{-19} \text{ C, } \frac{1}{4\pi\varepsilon_0} = 10^{10} \text{ V*m/C. (a), cos(x). (b), cos(0.1*x).} \]

In [19] we presented a method of calculation of the potential for a structure of arbitrary design, but periodic in one direction. We used the Bloch’s theorem for periodic medium with the aim of the Coulomb’s law simplification. The theorem allowed to get the wave function in periodic repeating medium in the form of a periodic function.

Using these results, we can calculate the map of the potential for the infinitely long, thin periodically charged thread. Let us write the charge distribution:

\[ \rho(x', y', z') = \lambda_0 \cos(kx')\delta(y', 0)\delta(z', 0) , \tag{4} \]
\[ \rho_c(x',y',z') = \lambda_0 e^{ikx'} \delta(y',0)\delta(z',0), \] 
\[ \rho(x',y',z') = Re\rho_c(x',y',z'), \]

where \( k \) is the crystal wave vector.

In [19] we expanded in a series the charge distribution:
\[ F^{(\rho)}_k(y',z'; G') = \lambda_0 \delta(y',0)\delta(z',0)\delta_{0,G'}, \] 
\[ F^{(V)}_k(y,z; G) = \frac{1}{4\pi \varepsilon_0} \lambda_0 \delta_{0,G} D_k(y',z'; G), \]

where \( G \) is the vector of reciprocal lattice, \( F^{(V)}_k(y,z; G) \) and \( F^{(\rho)}_k(y,z; G) \) are the coefficients of expansion for the potential and charge distribution respectively.

The electric potential can be presented in the form [19]:
\[ V_k(x,y,z) = \sum_G F^{(V)}_k(y,z; G)e^{i(k+G)x} = \frac{1}{4\sqrt{2\pi}^2 \varepsilon_0} \lambda_0 e^{ikx} D_k(y',z'; 0), \]

where \( D_k(y',z'; 0) \) is the integral
\[ D_k(y',z'; 0) = \int \frac{e^{ikx''}}{\sqrt{x''^2 + a^2}} dx''. \]

The calculation of the electric potential, obtained by expression (9) for the infinitely long, thin periodically charged thread, lying along the axis x is presented in figure 2. Here we also used the trapezoidal rule for calculation of the integral.

![Figure 2](image_url)

**Figure 2.** Distribution of the electric potential for \( \lambda_0 = 10^{-19} \text{ C}, \frac{1}{4\pi \varepsilon_0} = 10^{10} \text{ V*m/C}. \) (a), \( k = 0.1 \text{ nm}^{-1}. \) (b), \( k = 1 \text{ nm}^{-1}. \)

Further, we modified the algorithm of calculation of expression (9). We combined two algorithms for calculation of the first and second models. The new distributions is very different from the previous ones, that is shown in figure 3.
Figure 3. Distribution of the electric potential for $\lambda_0 = 10^{-19}$ C, $\frac{1}{4\pi \varepsilon_0} = 10^{10}$ V·m/C. (a), $k = 0.1$ nm$^{-1}$. (b), $k = 1$ nm$^{-1}$.

3. Conclusion
We have presented three methods of calculation of the potential for a periodic structure. The methods were applied for an infinitely long, thin periodically charged thread. They differ qualitatively – in the form of the potential distribution, and quantitatively – in the value of the electric potential. The first method has an unreliable value of the electric potential, but the second one has an unreliable form. The third method has the form of potential distribution from the first method and the value of the electric potential from the second method. Our findings are a step to understanding of how to build a map of the surface electric potential distribution for a periodic structure. It’s very important because photonic-plasmonic crystals have periodicity. The method can be useful for creating materials with necessary design and parameters.
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