Edge modes splitting by nanostructured surface

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Abstract. In this work the regularities of edge modes splitting in electrostatic approximation were considered in the structures like paraboloid of revolution. It was demonstrated that large splitting of edge modes occur within determined interval of wave vector with splitting out a soft, zero mode.

Nano-structured systems play a sufficient role in the miniaturizing process of devices in contemporary electronics as well as enable ones to include unusual properties of these objects into an arsenal of modern technology. Some attractive moment in nano-system usage is the circumstance that theirs properties, as a rule, are described by quantum physics laws what causes the appearance of new possibilities in realization more universal devices in addition to traditional ones.

In the present work effects that were connected with edge modes splitting by sharp formations on a nano-structured surface were studied. Analytical solution was carried out for the case of paraboloid of revolution. The problem was solved in the electrostatic approximation at the condition when wave length of incident electromagnetic radiation \( \lambda \) is more large than characteristic size \( L \) of scatterer, i. e. \( \lambda >> L \). Laplace’s equation was solved in parabolic coordinates \((\xi, \eta, \phi)\):

\[
\nabla^2 \Phi = \frac{1}{\xi^2 + \eta^2} \left[ \frac{1}{\xi} \frac{\partial}{\partial \xi} \left( \xi \frac{\partial \Phi}{\partial \xi} \right) + \frac{1}{\eta} \frac{\partial}{\partial \eta} \left( \eta \frac{\partial \Phi}{\partial \eta} \right) \right] + \frac{1}{\xi^2 + \eta^2} \frac{\partial^2 \Phi}{\partial \phi^2} = 0
\]

(1)

The solution is carried out by the traditional methods and looks like this:

\[
\Phi_{mq}(\xi, \eta, \phi) = \begin{cases} 
A_{mq} J_m(\sqrt{q}\xi) I_n(\sqrt{q}\eta) e^{im\phi}, & \eta \leq \eta_0, \ -\infty \leq \xi \leq \infty; \ 0 \leq \phi < 2\pi \\
B_{mq} J_m(\sqrt{q}\xi) K_n(\sqrt{q}\eta) e^{im\phi}, & \eta \geq \eta_0, \ -\infty \leq \xi \leq \infty; \ 0 \leq \phi < 2\pi 
\end{cases}
\]

(2)
where the conditions \( \eta = \eta_0, -\infty \leq \xi \leq \infty, 0 \leq \phi \leq 2\pi \) correspond to the border of paraboloid of revolution, \( q \) is a wave vector, \( J_m(\sqrt{q\xi}) \) is usual Bessel’s function, \( I_m(\sqrt{q\eta}), K_m(\sqrt{q\eta}) \) are Bessels’ functions of imaginary argument (Macdonald functions), \( m \) is a number.

The boundary conditions for the problem being solved were continuity of potential \( \Phi_{mq}(\xi, \eta, \phi) \) and derivation \( \varepsilon \partial_\eta \Phi_{mq}(\xi, \eta, \phi) \) on the border \( \eta = \eta_0 \) of paraboloid of revolution, where \( \xi, \eta, \phi \) are corresponding parabolic coordinates, \( \varepsilon \) is a dielectric constant of substance of paraboloid, an external medium was an air, \( q \) is a wave vector, \( m \) is a magnetic number, coordinate \( \eta \) describes “moving aside” of a base parabola. After demanding boundary condition being fulfilled for equation solution one can obtain in the case when some coefficients \( A_{mq} \) and \( B_{mq} \) are not equal to zero a dispersion correlation for electrostatic modes that are localized near the top of paraboloid:

\[
\varepsilon(\omega) = \frac{I_m(\sqrt{q\eta_0})}{I_m'(\sqrt{q\eta_0})} \frac{K_m'(\sqrt{q\eta_0})}{K_m(\sqrt{q\eta_0})}
\]

\[ (3) \]

**Figure 1.** Dispersion curves for dependence \( \omega/\omega_p \) versus \( X = \sqrt{q\eta} \) with splitting of soft, zero mode for dispersion law \( \varepsilon(\omega) = 1 - \omega_p^2/\omega^2 \) in the case of convex paraboloid of revolution (bottom part of the graph, numbering of modes rises from bottom), and ones with splitting of dispersion curve which is approached to the bulk plasmon for concave paraboloid (upper part of the graph) – (a). Splitting of dispersion curves for dependence \( \omega/\omega_p \) versus \( X = \sqrt{q\eta} \) for upper zones of convex (under \( \sqrt{\sqrt{2}} \)) and concave (above \( \sqrt{\sqrt{2}} \)) paraboloids for first four modes (b)

Putting dielectric constant for narrow band semiconductors (and high doped ones) in the form: \( \varepsilon(\omega) = 1 - \omega_p^2/\omega^2 \) one can obtain following result for dimensionless variable \( \omega/\omega_p \) for typical values \( n = 10^{23} \text{ cm}^{-3}, m^* = m_0 = 9.1 \cdot 10^{-28} \text{ g} \) which is presented on the Figure 1, where \( X = \sqrt{q\eta} \).

For determination of dispersion curves for concave paraboloid in the form of parabolic pit on a flat interface, for example, an air and semiconductor one should change in expression for \( \varepsilon(\omega) \) this value into \( \varepsilon'(\omega) \), what results from a demand of continuity of derivative with respect to corresponding variable quantities on the border of two media that are changed each other by places in this case. As a
result one can obtain dispersion curves that are presented on the Figure 1. Evaluation of maximal splitting region gives $\sqrt{q\eta} \leq 10$. The region of maximal splitting of edge modes for an upper band for $\lambda \sim 500$ nm has an order of 800 nm and the region of modes splitting spread up to approximately 8 $\mu$m.

The character of soft mode for a convex paraboloid of revolution in approximation $\bar{q} \to 0$ ($X = \sqrt{q\eta} \to 0$) is described by following formula:

$$\omega_0(\bar{q} \approx 0) = \frac{\omega_0}{\sqrt{2}}X \left[ \ln \left( \frac{2}{X} \right) \right]^{1/2}$$ (4)

In the work [1] an analogous result was obtained which was interpreted as a quasi-acoustical mode which has a dispersion law of one dimensional plasmon. Thus, soft, zero mode can be identified with collective plasmon excitation and generally speaking obtained in a corresponding way be means of polarization operator.

The special structures were prepared on the base of standard silicon wafers with specific resistance equals 4.5 Ohm-cm and (100) orientation. Then vertical columns were formed by plasma-chemical way by means of Bosch-process through chromium (Cr) mask with the thickness of 30 nm while using lift-off lithography. The result of described procedure is presented on the Figure 2.

Figure 2. Yellow colored structures (a), green colored structures (b), black colored structures (c), that were formed by plasmochemical etching on silicon wafer.

Drude–Lorentz–Sommerfeld model in the framework of which dispersion law $\varepsilon(\omega) = 1 - \omega_0^2/\omega^2$ was presented precisely enough describes optical properties in particular metals in infrared region. In visible region this model should be completed taking into account a response of binding electrons. Within frameworks of classical model it can be done by means of considering dielectrics or semiconductors as a sum of molecules each of them is an oscillator with the same resonant frequency $\omega_0$. The equation of motion for an electron in Drude–Lorentz–Sommerfeld model can be presented as following:

$$\frac{\partial^2 \vec{r}}{\partial t^2} + \Gamma \frac{\partial \vec{r}}{\partial t} + \omega_0^2 \vec{r} \approx \frac{e\vec{E}}{m} \exp(-i\omega t)$$ (5)

where $\vec{r}$ is a displacement of charge along $\vec{E}$ direction relatively non-perturbed location, $\omega$ is a frequency of incident radiation, $\omega_0$ is a frequency of a binding transition, $m$ is the mass of a free
electron, $\Gamma$ is a constant which is resulted from charge carrier relaxation, moreover, for the metals on the order $\Gamma$ is equal to $\Gamma = \upsilon_F / l$, $\upsilon_F$ is a velocity on a Fermi surface, $l$ is a free path length of charge carriers. Let us note that for free electrons last addend in the right hand side is absent so that $\omega_0 = 0$. To analyze the character of reflection spectra during interaction of radiation with free electrons one can use the expressions for real ($\varepsilon_r$) and imaginary ($\varepsilon_i$) parts in the form
\[
\varepsilon_r(\omega) = \varepsilon_\infty \left( 1 - \frac{\omega_p^2}{\omega^2 + \tau^2} \right); \quad \varepsilon_i(\omega) = \frac{\omega_p^2}{\omega^2 + \tau^2} \tau_p,
\]
where $\varepsilon_\infty$ is a high frequency dielectric constant, $\omega$ is a cyclic frequency of incident light, $\tau$ is a time between collisions, $\tau_p$ is a momentum relaxation time of charge carriers, $\omega_p$ is a plasmon frequency, $\Gamma = \tau^{-1}$. Taking into account formulae for $\varepsilon_r$ and $\varepsilon_i$ one can conclude that the result of calculations looks like that presented on the Figure 3 (we put approximately $\tau \sim \tau_p$).

For reflection coefficient at a normal fall of radiation following formula takes place
\[
R = \frac{(n - 1)^2 + \kappa^2}{(n + 1)^2 + \kappa^2},
\]
where $n$ is a refraction coefficient, $\kappa$ is absorption coefficient (extinction coefficient), moreover:
\[
n = \sqrt{\frac{1}{2} \left( \varepsilon_r + \sqrt{\varepsilon_r^2 + \varepsilon_i^2} \right)}; \quad \kappa = \sqrt{\frac{1}{2} \left( -\varepsilon_r + \sqrt{\varepsilon_r^2 + \varepsilon_i^2} \right)}.
\]  

\begin{figure}[h]
\centering
\includegraphics[width=0.4\textwidth]{figure3}
\caption{Dependence of refraction coefficient $R$ against the cyclic frequency $\omega$ of incident radiation in Drude–Lorentz–Sommerfeld model for free electrons at following values of parameters: $\omega_p = 5 \cdot 10^{14} \text{ s}^{-1}$, $\tau = 2 \cdot 10^{-14} \text{ s}$, $\omega_p = 8 \cdot 10^{14} \text{ s}^{-1}$, $\tau = 2 \cdot 10^{-14} \text{ s}$, $\varepsilon_\infty = 11.8$ – (2).}
\end{figure}

Near the minimum of dependences for wave-guidance modes the correlation takes place for the low mode: $\sqrt{q_{min}^2 \cdot \eta_0} \sim 1$, where $q_{min} = \frac{2\pi}{\lambda_{min}}$ corresponds to the minimum of dependence $\omega(q)$. Taking the value $\eta_0^2 \sim d_0 \sim 2r_0$ ($r_0$ is characteristic radius of coloring structure) one can obtain for estimations the proportional dependence ($\lambda_{min} \sim r_0$) for wave length which corresponds to the minimum on dispersion curve and for radius of curvature of scattering system. The mode with such a wave length will be captured more effectively by distorted surfaces.

References
[1] Longe P, Bose S M 1993 Phys. Rev. B. 48, 18239 – 18243