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On multi layers X-ray mirrors at about 100 eV on doped super lattice in *n*-Si nearby X-ray characteristic line

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Calculation of dielectric permittivity nearby X-ray characteristic line transition in degenerate *n*-Si is given. Possibility to fabricate multilayer X-ray mirror (MXM) nearby the transition with periodic n-doping with reflection coefficient up to about 50% at 77 K is demonstrated. It is pointed out possibility to produce dynamic masks in such MXMs via Shark effect in powerful optical radiation.

Keywords: X-ray emission, multilayer X-ray mirrors, X-ray characteristic line transitions.

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The fabrication of multilayer X-ray mirrors (MXMs) is a challenge for the future of Russian microelectronics. Cutting-edge research in this field is performed in Russia by our colleagues at the Institute for Physics of Microstructures of the Russian Academy of Sciences (see [1,2], references therein, and numerous reports in the proceedings of „Nanophysics and Nanoelectronics" symposia held at the Institute for Physics of Microstructures). Databases of X-ray characteristics (specifically, database [3]) are used for MXM design. The indicated database contains data on GaAs, Si, and SiO_2 materials and was used to construct MXMs in [1]. We use these data for evaluation, although technological issues are naturally omnipresent and affect the MXM parameters. At present, MXMs are produced by combining different materials, which often causes difficulties and, in certain cases, requires the use of a buffer between layers. Heavy metals form the basis of such MXMs. The permittivity of these metals in the X-ray wavelength range is affected most significantly by the non-resonance plasma contribution [4], and the resonance contribution of characteristic line transitions [5] is just an addition (cf. [1]). This approach allows one to tailor layer thicknesses to a given X-ray source frequency. If a single material is used, the problem of combining different layers becomes irrelevant, although the frequency is limited by a narrow resonance region of characteristic line transitions. In light materials (of which silicon is an example), the resonance contribution of characteristic line transitions is dominant. The leading part in construction of MXMs based on characteristic line transitions is played by the degeneracy of electrons in the upper band, where the edge of the Fermi distribution is a weak (logarithmic) resonance.

The aim of the present study is to demonstrate the feasibility of fabrication of an MXM with substantial reflectance based on a characteristic X-ray line transition and stimulate experimental research (including studies into the dynamic masks for such MXMs) in this field.

The energy spectrum of silicon consists of deep and almost discrete levels K, L, and M and upper bands. We consider the transition from level L (which is weakly split) to six electronic states of the conduction band (X-valleys). The mass of the density of states in valleys is $m_d = 0.32m_0$, and the mass of conduction is $m_c = 0.26m_0$, where m_0 is the mass of a free electron. The anisotropy of valleys is neglected. Figure 1 shows the transmission spectrum of silicon in the vicinity of the characteristic line transition (about 100 eV) frequency plotted based on the data from [3]. If one presents permittivity as $\varepsilon = 1 + \Delta\varepsilon$, where $\Delta\varepsilon = \Delta\varepsilon_1 - i\Delta\varepsilon_2$, it becomes evident that the transition comes into play at 100 eV, which leads to an increase in absorption and the emergence of imaginary part of permittivity $\Delta\varepsilon_2$. It follows from the data presented in [3] that $\Delta\varepsilon_2$ is 0.002 before the characteristic line transition and 0.02 at its peak. Real part $\Delta\varepsilon_1$ of permittivity

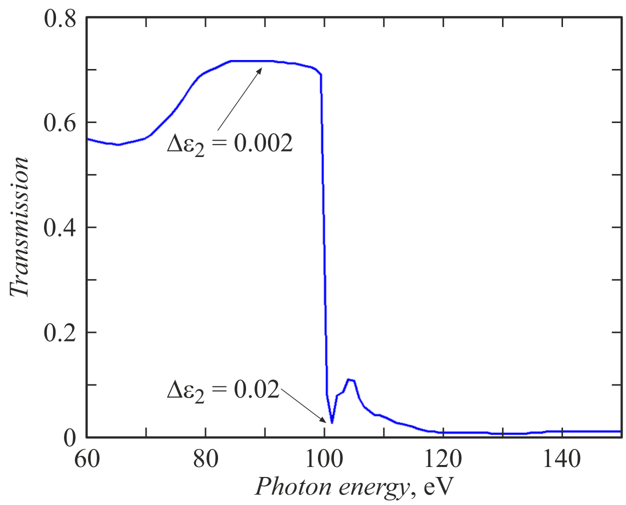

Figure 1. Transmission of a silicon wafer 0.2 μm in thickness [3]. The values of imaginary part $\Delta\varepsilon_2$ of the addition to unit permittivity are indicated.

is negative (plasma), but drops to a level below 0.001 on approach to the region of characteristic line transition energy around 100 eV, which is the one examined here.

The expression for addition $\Delta\varepsilon$ in weak field $E \propto \exp(i\omega t)$ [6] may be rewritten in the form used in laser physics (with a level population difference and a positive oscillator strength f^0_{lj}). In silicon, the sum over levels is the sum over wave vectors k of the Bloch functions, and the oscillator strength for a uniform electric field E has a delta function in k (the law of conservation of momentum). Thus, $\Delta\varepsilon$ for silicon takes the following form:

$$\Delta\varepsilon = \Delta\varepsilon_1 - i\Delta\varepsilon_2 = 2\cdot 6\frac{4\pi e^2}{m_c(2\pi)^3}\int d^3k \times \sum_{lj}\big(n_l(k) - n_j(k)\big)\frac{(f^0_{lj})^+}{\omega^2_{lj}(k) - \omega^2 + i\nu\omega}. \quad (1)$$

Here, factor 2 accounts for spin, 6 is the number of X-valleys considered individually, the sum over k is replaced by an integral, $n_l(k)$ and $n_j(k)$ are the band filling numbers, $(f^0_{lj})^+$ is the positive oscillator strength, and ν is the broadening of levels, which may also be reflective of incomplete degeneracy in the upper band. This expression describes the resonance contribution at the characteristic line transition frequency and the non-resonance contribution. The non-resonance contribution may be regarded tentatively as a plasma one $\big(\Delta\varepsilon \propto 1/(-\omega^2 + i\nu\omega)\big)$ only for those terms in (1) for which $\omega^2_{lj}(k) \ll \omega^2$. This actually implies that energy E_l of the lower level of the transition is smaller than frequency quantum ω: $\hbar\omega > E_l$ [4], since level energy $E_l \propto (Z/n)^2$ (n is the level number) and the energy of upper levels decreases as $1/n^2$. Silicon has nucleus charge $Z = 14$ and K-level energy $E_0 > 100$ eV; i.e., the contribution to $\Delta\varepsilon_1$ is positive for the transition from the K-level. The plasma contribution in silicon arises in non-resonance transitions from level L and in transitions from partially filled level M.

For the resonance contribution, we take only one term in (1), where the lower level is the L-level, which is considered to be unique and discrete with energy E_L. The upper level (band) is considered to be parabolic with effective masses of the density of states and conduction being m_d and m_c. Resonance $\Delta\varepsilon$ then takes the form

$$\Delta\varepsilon = \Delta\varepsilon_1 - i\Delta\varepsilon_2 = 2\cdot 6\frac{4\pi e^2}{m_c(2\pi)^3}\int d^3k\big(n_L(k) - n_B(k)\big) \times \frac{(f^0_{LB})^+}{\omega^2_{LB}(k) - \omega^2 + i\nu\omega}. \quad (2)$$

Here, k is measured from the bottom of an X-valley and

$$\omega_{LB}(k) = \frac{E^0_b - E_L + (\hbar k)^2/(2m_d)}{\hbar} = \omega_0 + \frac{\hbar k^2}{2m_d}.$$

Silicon may be doped with donors to concentration N around 10^{21} cm^{-3}. However, the concentration is spread over six valleys.

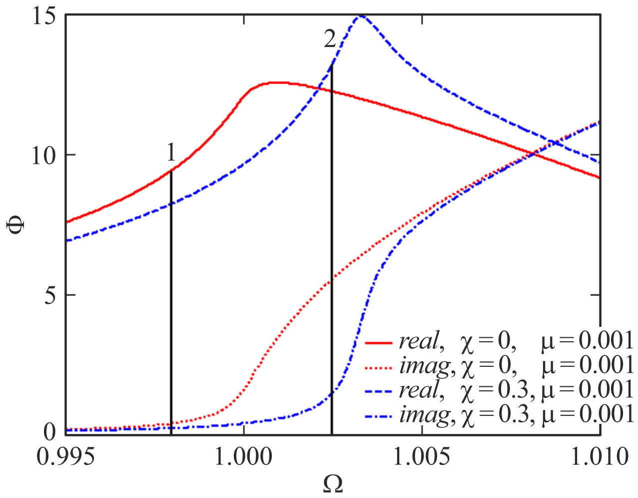

Figure 2. Dimensionless coefficient Φ in the addition to permittivity: the case of limit silicon doping with $N \approx 10^{21}$ cm^{-3} ($\chi = 0.3$) and narrow broadening ($\mu = 0.001$). Lines 1 and 2 denote dimensionless frequencies Ω at which reflection coefficient R was estimated: $R_1 \approx 0.35$ and $R_2 \approx 0.4$.

Let us integrate $\Delta\varepsilon$ in (2) over the solid angle in the k-region, take $(f^0_{LB})^+$ outside the integral sign, denote its mean as f_0, and introduce variables $x = k/k_B$, $\Omega = \omega/\omega_0$, $\gamma = [(\hbar k_B)^2]/\hbar\omega_0$, and $\mu = \nu/\omega_0$, where k_B is the boundary of the Brillouin zone. Under the assumption of complete degeneracy in bands (levels), $n_L(k) = 1$ at all k and $n_B(k) = 1$ at $k < k_F$. Since (2) contains difference $n_L(k) - n_B(k)$, the lower limit of integration over k is k_F. Setting $\chi = k_F/k_B$, we obtain

$$\Delta\varepsilon = \Delta\varepsilon_1 - i\Delta\varepsilon_2 = \Delta\Phi(\Omega, \chi, \mu), \quad (3)$$

$$\Delta = \frac{2\cdot 6}{(2\pi)^3}\frac{(4\pi e)^2 k_B^3 f_0}{m\omega_0^2}, \quad (4)$$

$$\Phi(\Omega, \chi, \mu) = \int_\chi^1 \frac{x^2dx}{(1+\gamma x^2)^2 - \Omega^2 - i\Omega\mu}. \quad (5)$$

Here, $\gamma = 0.036$ and $\Phi(\Omega, \chi, \mu)$ for various χ and μ are presented in Figs. 2 and 3. At an energy of 100 eV, $\Delta = 0.06 f_0$, $\max(\mathrm{Im}\,\Phi) = 19$, and $\max(\Delta\varepsilon_2) = 1.2 f_0$. According to [3], $\max(\Delta\varepsilon_2) = 0.02$, which yields $f_0 \approx 0.018$. Since six valleys are present, the Fermi energy in each valley is $E_F = \hbar^2/(2m(N\pi^2/2)^{2/3})$, where N is the overall concentration. At $N = 10^{20}$ cm^{-3}, we have $E_F = 0.065$ eV, $k_F = 8.22\cdot 10^6$ cm^{-1} $\chi = 0.143$; at $N = 10^{21}$ cm^{-3}, $E_F = 0.14$ eV, $k_F = 1.77\cdot 10^7$ cm^{-1} $\chi = 0.3$. Condition $E_F \gg kT$ needs to be fulfilled to establish degeneracy. Since nitrogen has $kT = 0.007$ eV, formulae (3)–(5) are valid at $T = 77$ K and $N = 10^{20}$ cm^{-3}.

The considered MXMs consist of layers of equal thickness of a quarter of a wavelength of undoped ($\chi = 0$ $(\Delta\varepsilon_n)$) and doped ($\chi = 0.3$ or 0.2 $(\Delta\varepsilon_l)$) silicon with sharp boundaries. To estimate reflection coefficient R of an

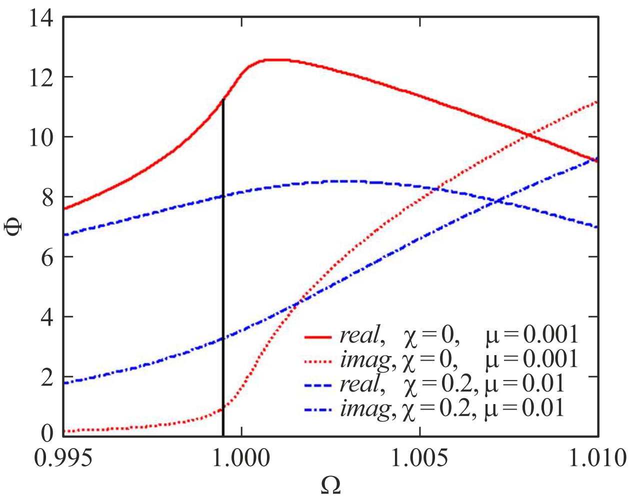

Figure 3. Dimensionless coefficient Φ in the addition to permittivity: the case of doped silicon with $N \approx 10^{20}\,\mathrm{cm}^{-3}$ ($\chi = 0.2$) and increased broadening ($\mu = 0.01$). The line denotes dimensionless frequency Ω at which reflection coefficient $R \approx 0.4$ of the proposed MXM was estimated.

MXM, we find the first harmonic A_1 of period $\Delta\varepsilon$ with difference $\delta\varepsilon$ in the layers. Denoting this difference as $\delta\varepsilon = \Delta\varepsilon_n - \Delta\varepsilon_l$, we obtain $A_1 = \delta\varepsilon/\pi$. Since our study should motivate further experimental research, we perform a simple evaluation of the reflection coefficient of the proposed MXMs. First, we determine absorption length L_d (by the X-ray wave amplitude) from absorption coefficient $\varsigma = \Delta\varepsilon_2 k/2 = 1/L_d$. Here, $\Delta\varepsilon_2$ is the sum of both non-resonance $(\Delta\varepsilon_2)_n$ (Fig. 1) and $\Delta\varepsilon_2$, which arises from $\delta\varepsilon$, since $\delta\varepsilon$ may also depend on $\Delta\varepsilon_2$. Note that the contribution of this $\Delta\varepsilon_2$ to L_d should be divided by 4 (and not by 2, as was done above in the expression for ς), since the contribution corresponds to a half of the MXM period. Assuming that the incident wave amplitude remains unchanged over L_d, we then find (using the method of perturbation in A_1) reflection coefficient R at an MXM thickness equal to L_d: $R = kL_d\delta\varepsilon/(2\pi)$. The values of R determined this way are presented in the captions to Figs. 2 and 3 together with the chosen MXM frequencies.

Figure 2 presents the case of limit silicon doping with $N \approx 10^{21}\,\mathrm{cm}^{-3}$ ($\chi = 0.3$) and narrow broadening ($\mu = 0.001$). In the region with $\Delta\varepsilon_2 = 0$, the Φ difference at a maximum is 2–2.5. This yields $\delta\varepsilon \approx 2.5 \cdot 10^{-3}$, and the value of L_d determined from losses outside of the characteristic line transition is $2\,\mu$m. The maximum possible value of R is then close to 0.35. At a frequency where $\Delta\varepsilon_2 \neq 0$ in an undoped layer and $\Delta\varepsilon_2 = 0$ in a doped layer (Fig. 2, frequency 2), $\delta\varepsilon = \delta\varepsilon_1 + i\delta\varepsilon_2$, $\delta\varepsilon_1 = (\Delta\varepsilon_1)_n - (\Delta\varepsilon_1)_l$, and $\delta\varepsilon_2 = (\Delta\varepsilon_2)_l$ (the second subscript corresponds here to the period layer). The Φ difference for frequency 2 in Fig. 2 at a maximum for $\delta\varepsilon_1$ is 2.5 while Φ for $\delta\varepsilon_2$ about 6; thus, $|\delta\varepsilon| \approx 6.5 \cdot 10^{-3}$. The absorption length here is $L_d = ((\Delta\varepsilon_{2n} + \delta\varepsilon_2/2)k/2)^{-1} = 0.8\,\mu$m, and $R \approx 0.4$. These R estimates may increase if non-resonance absorption is suppressed considerably at $T = 77$ K.

Figure 3 presents the case of doped silicon with $N \approx 10^{20}\,\mathrm{cm}^{-3}$ ($\chi = 0.2$) and increased broadening ($\mu = 0.01$). At $\Omega = 0.999$, the Φ difference at a maximum for $\delta\varepsilon_1$ ($\delta\varepsilon_2$) is 4 (close to 2); thus, $|\delta\varepsilon| \approx 6.5 \cdot 10^{-3}$. The absorption length here is $L_d \approx 1\,\mu$m, and $R \approx 0.4$. This R estimate may also increase at $T = 77$ K.

Thus, the feasibility of fabrication of MXMs based on a doped superlattice near X-ray characteristic line transition frequencies in *n*-Si at wavelengths around 12 nm was demonstrated. Calculated data revealed that a reflection coefficient up to 40% may be achieved in a superlattice of $\sim 200-400$ periods of 6 nm with layers of undoped and doped silicon. It was mentioned that the reflection coefficient may be increased further by cooling to 77 K. The width of the spectral interval where these estimates hold true (E_R) is below 1 eV. As a justification, we note that narrow-energy sources of X-ray radiation are available and the spectrum may (should) be narrowed in order to avoid degradation of numerous X-ray optical elements found in chip fabrication setups. At the same time, dynamic masks produced by pulsed optical radiation, which alters the electronic spectrum due to the high-frequency (optical) Stark effect and switches off MXM regions for the duration of an X-ray pulse, may be used in the narrow X-ray spectrum where the proposed MXM operates. The characteristic parameter specifying the spectrum shift by the Stark effect is energy $W = (e\Xi)^2/(2m\omega^2)$ of electron oscillations in the optical field, where Ξ is the optical field amplitude [7]. In the case of radiation with a wavelength of $1\,\mu$m and a power of 1 MW focused into a $3\,\mu\mathrm{m}^2$ spot, $W \gg E_R$.

This condition enables the use of dynamic masks with a duration of several nanoseconds (i.e., with an energy lower than 1 mJ), but even lower values are also feasible, since the reflection spectrum is narrow. In the considered MXM with $\chi = 0.2$, the plasma frequency is on the order of the frequency of radiation with a wavelength of $1\,\mu$m; therefore, the skin layer is greater than L_d. Such optical masks based on microelectromechanical systems (MEMS) could serve as an alternative to MEMS-based X-ray masks.

Naturally, the actual prospects for application of the proposed MXMs and dynamic masks still require analysis (in particular, in regards to the source of X-ray radiation). However, the possibility to construct both chips and mirrors in a single process technology appears tempting. It would definitely be instructive to grow and measure such MXMs in the X-ray region, starting with test superlattices with a small number of periods where the Stark effect may also be studied.

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Conflict of interest

The authors declare that they have no conflict of interest.

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