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The influence of an Si-SiON interface structure on dc-electric field induced second-harmonic generation (EFISH)

The results are reported of an analysis of the influence of the structure of an Si-SiO_xN_{1-x} interface on the d.c. electric field induced second-harmonic generation (EFISH). A model of quadratic nonlinear polarization for second harmonic generation (SHG) is analysed, where the SHG eficiency is given by [1,2,3]:

$$\frac{I_{2\omega}}{I_\omega^2} = \left| F_b(\omega) \left[ik(\omega)\chi^{(2)}_{b,\mathrm{anis}}(\omega)\cos 4\psi \int_0^\infty G(\omega,z)\,dz + ik(\omega)\chi^{(2)}_{b,\mathrm{is}} \int_0^\infty G(\omega,z)\,dz \right.\right.$$
$$\left.\left. + \chi^{(3)}_b(\omega) \int_0^\infty G(\omega,z)\varepsilon_{st}(z)\,dz \right] + F_s(\omega)\left[\chi^{(2)}_s(\omega) + \chi^{(3)}_s(\omega)\varepsilon_{st}(-0)\right] \right|^2 .$$

$\chi^{(2)}_{b,\mathrm{anis}}$, $\chi^{(2)}_{b,\mathrm{is}}$ are anisotropic and isotropic terms of bulk quadrupole second order susceptibilities of silicon, $\chi^{(3)}_b$—bulk dipole third-order susceptibilities, $\chi^{(2)}_s$, $\chi^{(3)}_s$—second and third order dipole susceptibilities of the Si-SiO_2 interface, ψ—azimutal angle, ε_{st}—d.c. electric field, $G(\omega,z) = \exp\{i(2k_z + K_z)z\}$—factor responsible for retardation and absorption effects inside silicon, k, K—fundamental and SHG complex wave vectors respectively, F_b and F_s take into account Fresnel factors for the SHG waves from the bulk and surface contributions respectively.

To take into account quantum confinement in an ultrathin SCR (space charge region), self-consistent calculations using a DFT (Density Functional Theory) approach [4] were carried out. The influence of an impurity segregation effect, spatial distribution of the O/N ratio, spatial and energy distribution of interface traps in the interface region Si-SiO_xN_{1-x} and spatial distribution of the fixed charge in the oxide on dc-electric field induced second-harmonic generation (EFISH) were analysed. The influence of these distributions on the capability of EFISH generation for probing the static electric field in the Si-SiO_xN_{1-x} interface region and the O/N ratio was evaluated. A comparison was made with the approach based on δ-approximation of the interface traps charge and fixed charge in the oxide [5].

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