Optical properties of highly doped ZnO:Al films deposited by ALD process on Si substrate in visible and near infrared region

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Today transparent conductive oxides (TCO) are materials of a great importance for development "transparent electronics" and photovoltaics, irreplaceable for flat panel displays and thin film solar cells. Zinc oxide doped with III-group elements is one of extensively studied nonexpensive TCO materials for indium-tin-oxide (ITO) substitution. Though electrical and optical properties of weakly doped ZnO films are widely known, it is of interest to determine optical constants ***n*** and ***k*** as well as optical mobility, plasma frequency and effective mass for highly doped ZnO:Al films from measurements of reflectance in visible and near IR wavelength range accompanied with electrical measurements.

Al-doped ZnO films with Al content from 0.5 to 7 at.% and thicknesses in the range 260-420 nm were deposited by ALD process. Accordingly to Hall effect measurements the carrier concentration, mobility and resistivity were in the range $(0.9\text{-}4)10^{20}$ cm^{-3}, 16-6 $cm^2/V{\cdot}s$, $(4.2\text{-}2.5)10^{-3}$ Ohm·cm, respectively. Measurements of reflectance in visible range were carried out at various incidence angles (10, 30, 50, 70°) by using p-polarized light what allow us to determine more carefully ***n***, ***k*** and thickness of films from fitting interference curves. The two models of Cauchy and Drude-Lorentz were used. At increasing aluminium content in ZnO film optical constant ***k*** also increases testifying to an absorption by free electrons at wavelength greater than 800 nm. IR reflectance spectra were measured in the range 1.6-25 μm with Fourier-transform spectrometer Bruker IFS-66. Fitting of these spectra allow us to estimate plasma frequency ω_p and damping constant γ_p which describe relaxation processes related to optical mobility (or in-grain mobility). At increasing carrier concentration ω_p increases from 2380 cm^{-1} for ZnO with 0.5 at.% of Al to 4985 cm^{-1} for ZnO with 7 at.% of Al. At the same time γ_p also increases from 995 to 1900 cm^{-1}. Using the Hall concentration we determined electron effective mass ***m**** . In our films it grows from $0.29m_0$ to $0.5m_0$ with increasing of Al content. Optical mobility estimated from $\mu=e/\gamma_p m^*$ was in the range 25-10 $cm^2/V{\cdot}s$. It was found that optical mobility is larger than Hall mobility. The estimated contribution of grain boundaries scattering into electron mobility is about 60%.

For ZnO films with 5 and 7 at.% of Al we observed in IR spectra the band at 12-16 μm that can be related to Al-O phonon modes. PL measurements carried out at room temperature (λ_{exc}=266 nm) demonstrate one emission peak at 376-379 nm and two ones in visible range at 560 and 700 nm. At increasing Al content in ZnO films UV near band edge emission line drastically diminishes, red line diminishes as well. So we observe passivation of some extrinsic defects localized on film surface.

In accordance with optical investigations we can see the decrease of mobility and increase of electron effective mass at increasing Al content. The primary scattering mechanism is the scattering on grain boundaries. So, it is necessary to find out technological parameters and post-growing treatment for a reduction this process.

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