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Optical properties of AlN/*n*–Si(111) films obtained by method of HF reactive magnetron sputtering

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The 0.45–0.5 μm thick AlN films on silicon single crystal *n*–Si(111) substrates with specific resistance (2–3)·10^{-3} $\Omega \cdot cm$ have been obtained by evaporation of an aluminium target in Ar/N_2 (1/3.5) gas mix using high-frequency magnetron sputtering. The surface morphology and optical properties of AlN/*n*–Si(111) films have been studied (reflection spectra in 200–750 nm range and in 1.4–25 μm one). The refractive index of the films in the 505–675 nm wavelength range is 2.13. The films obtained have been shown to be polycrystalline. The difference in the reflection band arrangement between films and crystal in IR region have been explained by the presence of mechanical tensile stresses and influence of heavily doped *n*–Si(111) substrates on IR reflection of AlN films.

Методом высокочастотного реактивного магнетронного распыления алюминиевой мишени в газовой смеси Ar и N_2 (соответственно 1:3,5) получены поликристаллические пленки AlN толщиной 0,45–0,5 мкм на подложках из монокристаллического кремния *n*–Si(111) с удельным сопротивлением (2÷3)·10^{-3} Ом·см. Исследовано морфологию поверхности и оптические свойства пленок AlN/*n*–Si(111) (спектры отражения в диапазоне 200–750 нм, спектры отражения в диапазоне 1,4–25 мкм). Полученное значение показателя преломления пленок AlN/*n*–Si(111) в диапазоне длин волн 505–675 нм равно 2,13. Разница в размещении полосы отражения пленок и кристалла в ИК области спектра объяснена наличием механических напряжений растяжения и влиянием сильнолегированных подложек *n*–Si(111) на ИК отражения пленок AlN.

1. Introduction

The wideband aluminum nitride (AlN) has the bandgap value (E_g = 6.28 eV) exceeding considerably those for germanium, silicon, gallium arsenide, silicon carbide, gallium nitride and solid solutions of aluminum and gallium nitrides. Besides, AlN shows high values of the break-down critical electric field, high radiation stability, mechanical and thermal strength. The development of light emitting devices for visible spectral range is possible on its base. Up to now, there are no intrinsic substrates for AlN and its growth is realized by heteroepitaxy using substrates of other materials, including silicon [1–7].

In this work, AlN films were obtained on the heavily doped *n*–Si(111) substrates and the influence of such substrates on film growth and optical properties (because the doping is a method to control a device characteristics) was investigated.

2. Experimental

The AlN films were obtained by HF magnetron sputtering of aluminum target in Ar/N_2 gas mixture (1:3.5, respectively) using a modernized "Cathode 1M" installa-

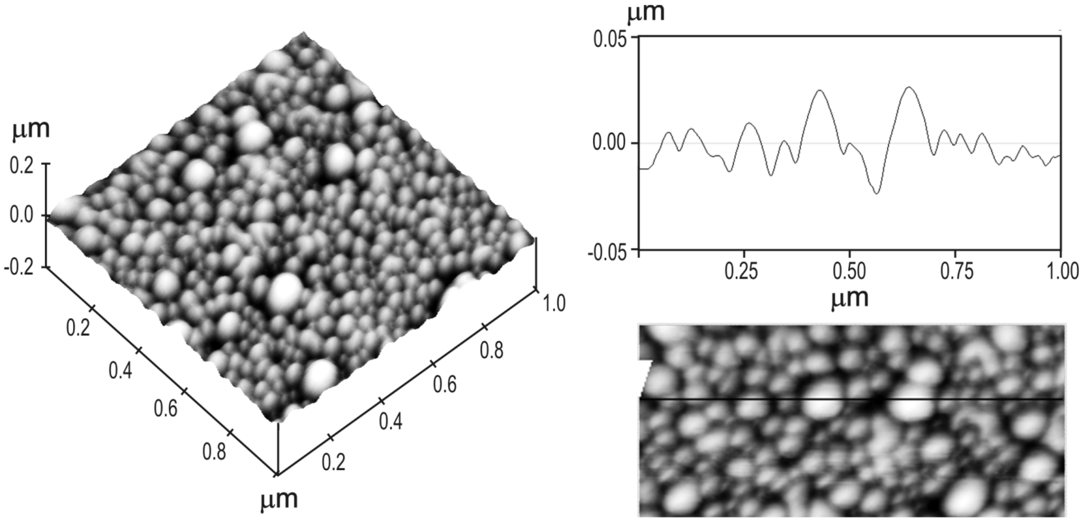

Fig. 1. Surface image of AlN film on n–Si(111) substrate with specific resistance $(2-3)\cdot10^{-3}$ Ω·cm.

tion (13.56 MHz frequency was used). The pressure value Prior to the process onset, the chamber was evacuated down to $1.33\cdot10^{-3}$ Pa by a TM-1000 oil-free turbomolecular pump. The total pressure in chamber during the process amounted 5.6 Pa. In order to obtain a more structured film, high-frequency discharge power amounted about 700 W (target diameter 16 cm). The film thickness was controlled during deposition onto the substrate by deposition rate which amounted 1.5 to 3 nm/min. The obtained AlN films were 0.45–0.5 µm thick. After the deposition completion, the thickness was controlled using an interferometer (MII-4). Silicon of electron type n–Si(111) with the resistivity of $(2-3)\cdot10^{-3}$ Ω · cm (electron concentration $2.5\cdot10^{19}$ cm^{-3}) was used as a substrate. Prior to the film deposition, the substrates were chemically etched. Chemical analysis of film composition were performed by secondary ion mass-spectrometry. The substrate surface and film morphology was investigated using an ACM Nanoscope IIIa Dimention 3000 (Digital Instruments, U.S.A.) in the periodic contact mode. The measurements were carried out in the central zone of the sample using commercial silicon probes (NT-MDT, Russia).

3. Experimental results

The surface morphology studies of n–Si(111) substrates have shown that the silicon surface is typical of the polished single crystal plates. The surface of AlN film is formed by separate homogeneously arranged islands of 40 to 80 nm in diameter and from 10 to 20 height, respectively. Among those, larger islands can be seen (100 to 150 nm diameter and 45 nm average height) at a density up to 10 per µm^2 (Fig. 1).

To obtain information on optical properties of the prepared films, the reflection spectra were measured in the 200–750 nm spectral range (MDR-23 diffraction grating monochromator) for the n–Si(111) substrate and AlN/n–Si(111) film (Fig. 2a, b). An interference pattern is observed for the reflection curve of AlN/n–Si(111) film (Fig. 2a,b, curve *2*). The well-known relations [8] can be used to estimate the values of optical parameters:

$$m\lambda_1 = 2n_1(\lambda_1)d, \tag{1}$$

$$(m+1)\lambda_2 = 2n_2(\lambda_2)\cdot d, \tag{2}$$

where m is the order of interference pattern; λ_1 and λ_2, wavelengths corresponding to the neighboring minima or maxima, respectively; d, the film thickness; $n(\lambda)$, refractive index of the film. From (1) and (2), it is possible to obtain interrelation between the film thickness d and refractive index of the film n:

$$d = \frac{\lambda_1\cdot\lambda_2}{2\left[n_2(\lambda_2)\cdot\lambda_1 - n_1(\lambda_1)\lambda_2\right]}. \tag{3}$$

Neglecting the refractive index dispersion in the λ_1 and λ_2 wavelengths interval, it is possible to write

$$n = \frac{\lambda_1\cdot\lambda_2}{2d(\lambda_1-\lambda_2)}. \tag{4}$$

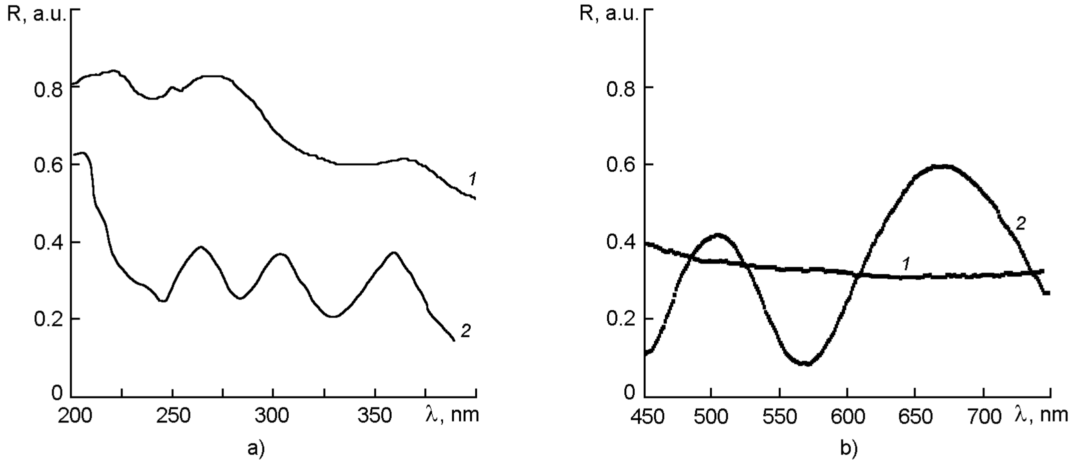

Fig. 2. Reflection spectra for n–Si(111) substrate (1) and AlN/n–Si(111) film (2).

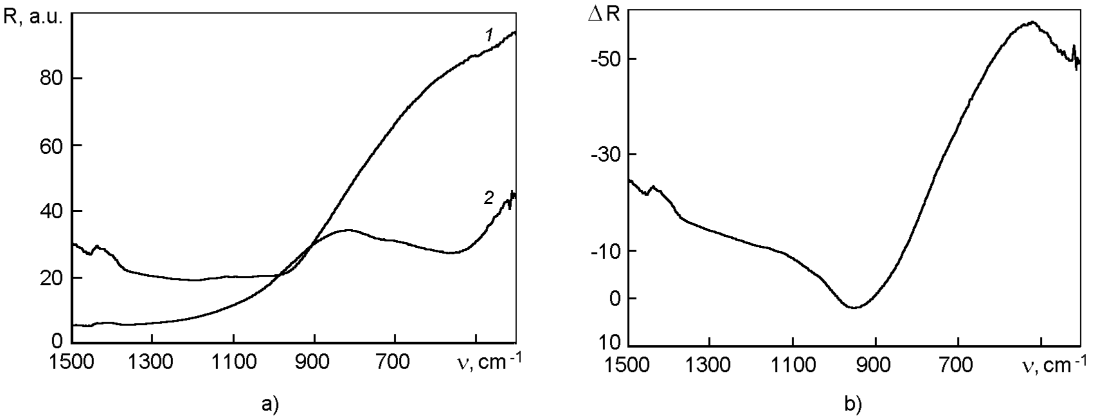

Fig. 3.(a) Frequency dependence of reflection for n–Si(111) substrate (1) and AlN/n–Si(111) film (2); (b) difference reflection spectrum of film and substrate.

The refractive index value for AlN/n–Si(111) film in the wavelength range 505–675 nm (neighboring maxima) obtained according to Eq.(4) and Fig. 2b is 2.13. As is seen from Fig. 2a, in the area close to 200 nm the reflectance coefficient increases (long-wavelength absorption edge for AlN is near $\lambda = 200$ nm).

The reflection spectra of n–Si(111) substrates (Fig. 3a, curve 1) and AlN/n–Si(111) films (Fig. 3a, curve 2) in the 1.4–25 μm range (Spectrum BXII IR Fourier spectrometer) have shown that a characteristic absorption band is observed in the film IR spectrum which is due to the TO-vibrations of the Al–N bonds. The position of the absorption band minimum corresponds to 547 cm^{-1} frequency (for crystals, this frequency is 610 cm^{-1} [9]). The difference in the absorption minima for the given film is explained by the distribution of the bonds and angles between them characteristic for this film, presence of mechanical tensile stresses (lattice constant of Si $a = 0.543$ nm and AlN, $a = 0.311$ nm, $c = 0.498$ nm, [1] are different, thus, at the onset of AlN film growth on the n–Si(111) substrate, mechanical stresses at the substrate/film interface arise, which are relaxed as the growth proceeds) and influence of the heavily doped n–Si(111) substrate on the IR-reflectance of AlN film.

In the spectrum of n–Si(111) substrate — (Fig. 3a, curve 1), plasma frequency is observed ($\omega_p = \left[e^2N/\varepsilon\varepsilon_0 m^*_{opt}\right]^{1/2}$, where $\varepsilon = 11.9$ [1], $\varepsilon_0 = 8.854\cdot10^{-12}\Phi/\mathrm{m}$, $m^*_{opt} = \dfrac{3m_{\parallel}\, m_{\perp}}{m_{\perp}+2m_{\parallel}}$, where $m_{\parallel} = 0.92m_0$ [10], $m_{\perp} = 0.19m_0$ [10]), which amounts 855 cm^{-1}. It can be seen from Fig. 3a, curve 1, that the reflectance minimum of n–Si(111) substrate is near 975 cm^{-1}. If we take specific resistance ρ equal to $2.5\cdot10^{-3}$ $\Omega\cdot\mathrm{cm}$, it is possible to estimate the electron mobility μ_e as 109.85 $\mathrm{cm}^2/\mathrm{V\cdot c}$. The phenomenological parameter of reflectance spectrum broadening for substrate ($\Gamma = e\hbar(\mu_e m^*_{opt})^{-1}$ [11]) is $4.085 \cdot 10^2$ eV. Because the main mechanism of the free charge carrier scattering is the scattering on the charged impurities, then relaxation time τ_i ($\tau_i = \hbar/\Gamma$) is $1.611 \cdot 10^{-14}$ s. It is to note that relaxation time on impulse τ_p estimated from data on reflectance spectrum of *n*–Si(111) substrate (Fig. 3a, curve *1*) using the Drude formula is of the same order.

In Fig. 3b, the difference reflectance spectrum (R_2–R_1, where R_1 is reflection of *n*–Si(111); R_2, reflection of AlN/*n*–Si(111) film), that evidences the predominant contribution from the substrate into total reflection capability of the external medium-film-substrate system.

4. Conclusions

Thus, the investigations of the surface morphology and optical properties of AlN/*n*–Si(111) films (reflectance spectra in 200–750 nm range and in 1.4–25 μm one) have shown that obtained films using HF magnetron sputtering are polycrystalline. The refractive index of the films in the 505–675 nm wavelength range is 2.13. The arrangement difference of reflection band between films and crystal in IR region are explained by the presence of mechanical tensile stresses and influence of heavily doped *n*–Si(111) substrates on IR reflection of AlN films.

References

1. P.Yu, M.Cardona, Fundamentals of Semiconductors. Springer, Berlin, 1996; P.Yu, M.Cardona, Principles of Semiconductor Physics, Fizmatlit, Moscow (2002) [in Russian].
2. Abstr. of 3rd Russian School of Scientists and Young Specialists on Physics, Material Science and Manufacturing Technology of Silicon and Device Structures Based Thereon "Silicon. School 2005", July 4–7, 2005, MISIS, Moscow (2005).
3. A.A.Lebedev, V.E.Chelnokov, *Fiz. Tekhn. Poluprov.*, **33**, 1096 (1999).
4. M.C.Luo, X.L.Wang, J.M.Li et al., *J. Cryst. Growth*, **244**, 229 (2002).
5. H.-E.Cheng, T.-C.Lin, W.-C.Chen, *Thin Sol. Films*, **425**, 85 (2003).
6. M.A.Auger, L.Vazquez, M.Jergel et al., *Surf. and Coat. Tech.*, **180–181**, 140 (2004).
7. C.H.Lai, A.Chin, B.F.Hung et al., *IEEE Elec. Dev. Lett.*, **26(3)**, 148 (2005).
8. T.Moss, G.Burrel, B.Ellis, Semiconductor Opto-electronics, Halsted Press, New York. (1973); T.Moss, G.Burrel, B.Ellis, Semiconductor Opto-electronics, Mir, Moscow (1976) [in Russian].
9. V.Y.Davydov, Y.E.Kitaev, I.N.Goncharuk et al., *Phys. Rev. B*, **58**, 12899 (1998).
10. A.I.Anselm, Introduction to the Theory of Semiconductors, Nauka, Moscow (1978) [in Russian].
11. A.M.Evstigneev, P.A.Gentsar, S.A.Grusha et al., *Fiz. Tekhn. Poluprov.*, **21**, 1138 (1987).

Оптичні властивості плівок AlN/*n*–Si(111), отриманих методом високочастотного реактивного магнетронного розпилення

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Методом високочастотного реактивного магнетронного розпилення алюмінієвої мішені у газовій суміші Ar і N_2 (відповідно 1:3,5) отримано полікристалічні плівки AlN товщиною 0,45–0,5 мкм на підкладках із монокристалічного кремнію *n*–Si(111) з питомим опором (2÷)·10^{-3} Ом·см. Досліджено морфологію поверхні та оптичні властивості плівок AlN/*n*–Si(111) (спектри відбивання у діапазонах 200–750 нм та 1.4–25 мкм). Отримане значення показника заломлення плівок AlN/*n*–Si(111) у діапазоні довжин хвиль 505–675 нм дорівнює 2.13. Різницю у розміщенні мінімуму смуги відбивання плівок та кристала в ІЧ області спектру пояснено наявністю механічних напружень розтягу та впливом сильнолегованої підкладки *n*–Si(111) на ІЧ відбивання плівок AlN.