

Epitaxial growth and properties of II_3V_2 semiconductors: Mg_3N_2 and Zn_3N_2

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The II_3V_2 semiconductors are a little-explored class of semiconductor materials which can be composed of environmentally-benign, earth-abundant elements, and have bandgaps in the visible and near infrared part of the spectrum. The crystal structure of these materials is relatively complex consisting of three interpenetrating fcc lattices, with one of the lattices half occupied. Epitaxial zinc nitride [1] and magnesium nitride [2] thin films were grown on (110) sapphire and (200) MgO substrates by plasma-assisted molecular beam epitaxy with nitrogen gas. The Mg_3N_2 and Zn_3N_2 films were grown at temperatures of 300-350°C and 140-180°C respectively. The RHEED pattern during growth and the x-ray $\theta/2\theta$ scans suggest that the films are epitaxial single crystals. In situ optical reflectivity during growth was used to determine the growth rate as a function of the metal flux and the growth temperature. The in-situ reflectivity was simulated by an optical model from which we derived the growth rate (up to 0.05 nm/s) and the indices of refraction of the deposited Mg_3N_2 and Zn_3N_2 films at 488 nm (2.4 and 2.65 respectively). X-ray diffraction shows that the thin films were (400) oriented on both the (110) sapphire (Zn_3N_2 only) and (200) MgO substrates. The optical absorption coefficient was calculated from the transmittance spectrum; the optical band gap of the Mg_3N_2 and Zn_3N_2 thin films were found to be 1.3 eV and 2.5 eV, respectively. Ellipsometry measurements show that the refractive index of zinc nitride is 2.3-2.7, and extinction coefficient is ~ 0.5 -0.7 in the energy range of 1.5-3.0 eV. The index of refraction of Zn_3N_2 has the unusual characteristic of decreasing with photon energy in the 1.7-3.0 eV range, whereas the index of Mg_3N_2 shows a normal dispersion with photon energy. The electron transport measurement shows that the single crystal zinc nitride has an electron mobility as high as 395 cm^2/Vs . Both materials are air sensitive and uncapped films oxidize in room air, especially Mg_3N_2 films which oxidize fully in minutes.



Figure 1. Photograph of capped Mg_3N_2 film 800 nm thick with chemical formula visible on paper below.

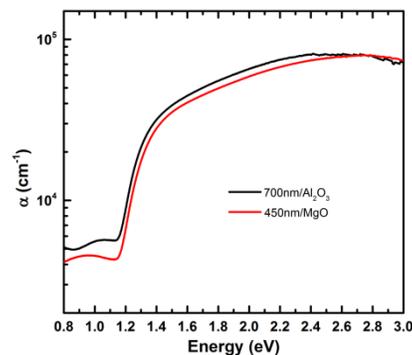


Figure 2. Optical absorption spectra of Zn_3N_2 films.

1. Peng Wu et al, *Semicond. Sci. Technol.* **31**, 10LT01 (2016)
2. Peng Wu et al, *Appl. Phys. Lett.* (submitted 2018)

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