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Synthesis and Applications of $Al_xGa_{1-x}N$ Semiconductor thin Films in Optoelectronic Devices.

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Abstract: $Al_xGa_{1-x}N$ thin films were deposited on ultrasonically cleaned glass substrates by thermal evaporation technique in a vacuum of about 2ա10 torr. X-ray diffraction, Raman spectroscopy, and SEM (scanning electron microscope) were used to characterize nanocrystalline thin films. X-ray diffraction study showed that, all the films have the hexagonal wurtzite structure, with lattice constants a=b=4.142, c=6.724A˚. Crystallite sizes calculated from Scherrer relation are in the range of 54.83-62.93 nm. Raman spectroscopy showed that the product were hexagonal wurtzite CdS with the 1st and 2nd harmonic modes at 300.1 and 601.34 cm-1 respectively. The optical properties of the nanocrystalline were investigated by the UV-VIS-NIR absorption spectroscopy. The band gap of the films was found to be 2.42 eV.

Keywords: $Al_xGa_{1-x}N$ Band gap, Thermal evaporation, Nanometer grain size, Raman spectroscope.

1.Introduction

Thin films of AlxGa1-xN are of great interest for their efficient use in the fabrication of solar cells [1, 2] and other optoelectronic devices [3]. There exists a vast literature [4-8] comprising of experimental and theoretical investigations of electronic band structure and related properties of this compound. The study of optical constants of AlxGa1-xN near the fundamental absorption edge is interesting in view of the importance of this material as a "model" photoconductor. Moreover, the study of optical constants in the sub band gap region is often of interest for using this material in solar cells and in other optoelectronic device designs. Accurate knowledge of the refractive index and absorption coefficient of semiconductors is essential for the drawing and analysis of various optoelectronic devices. While there have been many reports on the optical constants of AlxGa1-xN**,** the current state of available data in the visible to ultraviolet region seems to be less than adequate especially in the framework of structural phase transition in thin films.

Several workers have studied the optical properties of AlxGa1-Xn films deposited by different techniques like chemical bath deposition (CBD) [9], thermal evaporation [10], molecular beam epitaxy (MBE) [11] etc. Though by epitaxial techniques, it is possible to grow AlxGa1-xN thin films of single phase (either as cubic or hexagonal), generally a mixed phase for the films are obtained when CBD or by thermal evaporation is adopted. We have adopted thermal evaporation technique because of its simple and economic nature for the synthesis of AlxGa1-xN thin films. The AlxGa1-xN thin film so obtained has been characterized using the XRD, SEM, Raman spectroscopy and UV-VIS absorption spectroscopy.

2. Experimental section

AlxGa1-xN material was purchased from Alfa Aesar Company of United Kingdom. AlxGa1-xN films were deposited on well cleaned glass substrates by thermal evaporation technique. X-ray diffraction patterns, SEM images and optical absorption spectra were obtained using x-ray diffractometer (Philips Analytical-PW3710), scanning electron microscope (JSM-6380) and Jasco V-570 UV-VIS-NIR spectrophotometer, respectively. X-ray diffractometer was operated at 35kV and 30 mA with Cu KĮ radiation of wavelength 1.5406 A˚. Absorbance spectra were recorded in the range of 190-900 nm. The Raman spectroscopy of the films was performed using a Horiba

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Jobin Yvon laser Spectrometer 64000 and Olympus Inverted Microscope with Ar-ion laser at room temperature.

3. Results and Discussion

3.1 X-ray Diffraction Analysis

XRD pattern of AlxGa1-xN thin film deposited on glass substrate by thermal evaporation technique is shown in Fig. 1, which depicts that the film has a polycrystalline structure having hexagonal phase, with a (002) preferred orientation and shows a highly intense peak at ş=26.420. The grain size (D) values are calculated using the Scherrer formula [12],

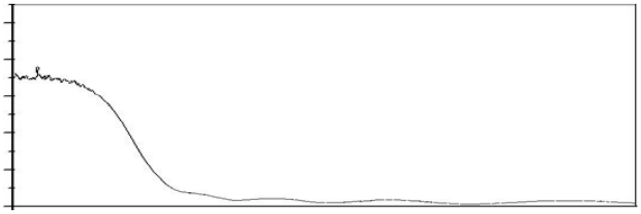

Fig.1: XRD of AlxGa1-xN thin Film Deposited on Glass Substrate.

3.2 Optical Properties

Optical absorbance and transmission spectrum of AlxGa1-xN thin films deposited on ultrasonically cleaned glass substrate are shown in Fig. 2 and Fig. 3, respectively. All films show good transmission for wave length larger than 500 nm which is one of the prerequisites for optoelectronic devices, especially for solar cell window layers [14]. Transmittance of thin films increases with wavelength, while rise and fall in the transmittance is observed for a longer wavelength. These types of variations are recognized to be due to the interference of light transmitted through the thin film and the substrate. Similar behaviors in the transmission spectrum of the AlxGa1-xN thin films prepared by other techniques have been reported earlier [6,15,16]. The transmission spectrum depicts a sharp fall in transmission near fundamental absorption, which is a typical indication of the good crystallinity of the films. In semiconductors, the relation connecting the absorption coefficient Į, the incident photon energy hĬ and optical band gap Eg takes the form

$$ĮhĬ = A (hĬ - Eg)p \quad (1)$$

Where k is constant related to the effective masses associated with the bands and p=1/2 for a direct material, 2 for an indirect material and 3/2 for a forbidden –direct energy gap. Since better linearity was obtained in the (ĮhĬ)2 vs. hĬ plot, the direct band gap values were determined by extrapolating the linear portion of these plots to the energy axis. The estimated Eg values are in the range 2.40-2.42eV, which are comparable to the values reported elsewhere [13].

3.3 Raman shift

Raman spectrum of AlxGa1-xN thin films deposited on glass substrate at room temperature is shown in Fig. 2. Strong fundamental and weak overtone modes are detected at 300.1 and 601.34cm-1, respectively. The fundamental and overtone modes correspond to the 1LO (longitudinal optical) and 2LO Peaks and are the result of phonon vibration [17-20]. These vibrations match well with vibrations of hexagonal wurtzite structure of AlxGa1-xN thin films reported at 297.0 cm-1 and 597.1 cm-1 by Thongtem et. al [21].

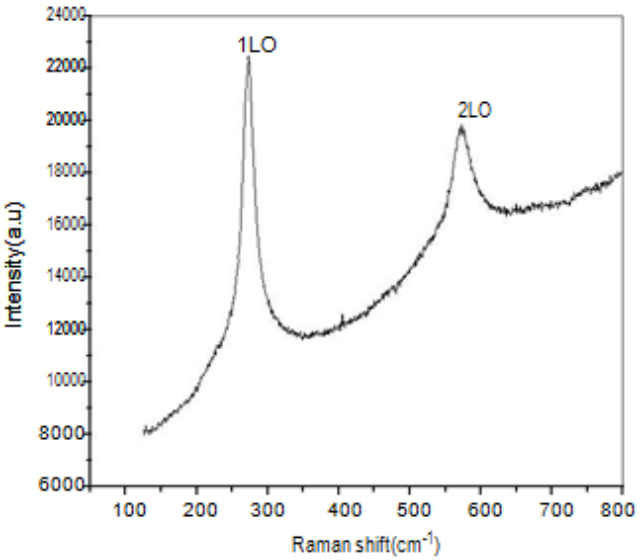

Fig. 2: Raman Spectrum of AlxGa1-xN thin Films Deposited on Glass Substrate.

3.4 D. SEM analysis

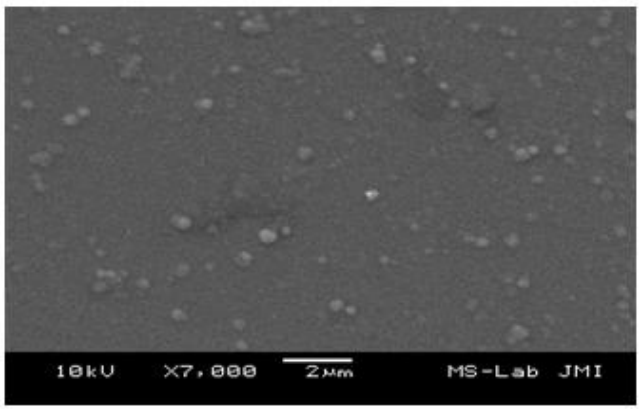

Fig. 3: SEM Micrograph of AlxGa1-xN thin Films Deposited on Glass Substrate.

Scanning electron microscopy is a convenient technique to study the microstructure of thin films. Fig. 3 displays the SEM micrograph of AlxGa1-xN thin films deposited at room temperature. It is observed that the deposited films are without any void, pinhole or cracks and cover the

substrate well [22]. The small nano-sized grains, like small spheres on plane sheet, are clearly observed in the micrograph, which clearly indicates the nanocrystalline nature along with some amorphous phase of AlxGa1-xN in the thin films. It is also observed that the nucleation was not uniform throughout the films and hence some cluster formation is also seen in the SEM micrograph. Grain size as estimated from the SEM is of the order of few hundred nm, far larger than the values obtained using the XRD data. Such a high difference may be due the some amorphous phase along the predominant nucleation [23]. Our main focus is the growth of compound semiconductor thin films, and understanding their optical and carrier transport properties with the aim of engineering better power and external quantum efficiencies in solid state lighting and solar cell applications, along with higher switching speeds and lower power consumption for transistor applications. We routinely use photoluminescence, photoluminescence excitation, electroluminescence, excited state lifetime, power efficiency, quantum efficiency, current-voltage, capacitance-voltage, residual potential and temperature dependent Hall measurements to study the electro-optical properties of our materials $Al_xGa_{1-x}N$ and devices (alternating current thin film electroluminescence, inorganic light emitting diodes, solar cells, organic light emitting diodes and thin film transistors).

4. Conclusion

In this work we have studied the optical and structural properties of AlxGa1-xN thin films obtained by the thermal evaporation technique. From XRD pattern grain size of AlxGa1-xN thin films is found to be 54.83-62.93 nm. SEM studies show irregular distribution of particles with cluster formation, having sizes of the order of few hundred nm. The films were found to have high transmittance of about 70 and 85% in the UV-VIS-NIR regions; hence they could be used as thermal control window coatings for cold weather and antireflection coatings. The films have a direct band gap of 2.42 eV.

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