Study of growth, composition and optical properties of as-deposited and post-treated a-SiNx:H thin films

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Institute, Year: Indian Institute of Technology Delhi (**2014**)

Silicon nitride thin films have been of interest since the advent of the microelectronics revolution. It has been traditionally used for diverse applications like dielectric gate material, impurity barriers, surface passivation, device encapsulation and optical coatings. Recently, the discovery of the Quantum Confinement Effect in Si nanocrystals in porous Si has led to interest in systems involving nano-dimensional silicon. Si quantum dots embedded in a silicon nitride matrix is one such system that is being explored towards applications in third generation solar cells and LEDs. These Si nanostructures are generally obtained by the process of phase separation in a silicon rich silicon nitride. The composition and microstructure of these films play a crucial role in determining the properties of these films. These factors are in turn strongly dependent on the deposition conditions and technique used. Plasma enhanced chemical vapour deposition (PECVD) has been a widely used technique for the silicon nitride thin film deposition. The films deposited by this technique have process induced hydrogen incorporated in them (therefore represented as *a*-SiN_x:H),which has a profound impact towards films' properties. Realizing the importance of these interrelated factors viz. composition, microstructure and the hydrogen content, the present thesis aims to study the dependence of properties, like photoluminescence and photoconductivity, on these factors. It also discusses the effect of various post-treatments like thermal annealing, rapid thermal annealing and swift heavy ion irradiation in terms of these crucial factors. It must be noted that these post-treatments are currently of intense interest towards useful harnessing of the quantum confinement related properties.

The thesis starts with investigation of the depth resolved chemical composition of a-SiN_x:H films by the novel technique of resonant soft X-ray reflectivity (R-SoXR). Such depth resolved composition determination allows for the comparison of the growth kinetics in films deposited under different deposition conditions. It is demonstrated that the depth compositional sensitivity (few nanometers) and non-destructive nature give R-SoXR a significant edge over the conventional composition determination tools like RBS and XPS.

The origin of luminescence from Si quantum dots embedded in dielectric matrix has been under constant debate. This ambiguity is inherent in the composite nature of these materials, for e.g. in silicon rich silicon nitride the presence of various radiative defects, bandtail luminescence as well as the quantum confined luminescence lead to difficulty in assigning the origin of luminescence. We demonstrate that investigation of the photoluminescence of these films with three excitation lasers can throw light on the radiative processes in these films. A deconvolution procedure is adopted which explains all PL spectra presented here. Further an interesting optical metastability is revealed in silicon rich silicon nitride, wherein a preferential enhancement of the PL band associated with Si inclusions in silicon nitride films is observed upon a low temperature exposure to atomic hydrogen. The preferential enhancement of PL is then used to investigate the variation of defect density in silicon rich silicon nitride with increasing Si content. The three laser approach for optical investigations is successfully applied to understand the effect of various post treatments on optical properties.

Further, the microstructural changes in silicon rich silicon nitride under swift heavy ion irradiation are presented. The nanostructuring of materials by the use of swift ions is receiving enormous interest. In the same area, ion tracks formation in various materials is being investigated vigorously. The present work reports for the first time the formation of discontinuous tracks in *a*-SiN_xH thin films through cross-sectional transmission electron microscope investigations. This nanostructuring of *a*-SiN_x:H holds great promise towards realisation of size and spatial control over the growth of Si QDs in silicon nitride.

With the emergence of the third generation solar cell concepts, the recent past has also seen a surge in interest in Si quantum dots embedded in dielectric matrices. The final chapter therefore addresses the photocurrent spectral response measurements on *a*-SiN_x:H of which only scarce reports exist in the literature. The narrow band UV response found in these films is quite unique to this class of materials and can be useful towards achieving third generation solar cell goals.

Note: The author is currently a researcher at the Nanoscale Research Facility of IIT Delhi (2014).