Study of Phase Evolution, Interfacial and Optical Properties of Amorphous Silicon Nitride Thin Films

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The exploration of a suitable dielectric matrix for Si-nanostructures which are known to exhibit efficient luminescence is of great interest for the realization of integration of optoelectronic devices with Complementary Metal-Oxide-Semiconductor (CMOS)-compatible Si technology. In this regard, hydrogenated amorphous silicon nitride (*a*-SiN_x:H) has been actively explored as an alternative dielectric matrix, due to its low potential barrier and efficient emission at shorter wavelengths. However, as *a*-SiN_x:H thin films are generally deposited by CMOS-compatible Chemical Vapour Deposition(CVD) techniques using silane (SiH_4) and ammonia (NH_3) as the precursor gases, the inadvertent incorporation of hydrogen and oxidation of these films demand optimization of various parameters to stabilize the desired phase(s). Moreover, control and uniform size distribution of Si-nanostructures still remain a concern for the scientific community.

The main aim of the present thesis is to study the relevance of hydrogen in evolution of various phases and their stabilization in the as-deposited (ASD) and post-deposition treated a-SiN_x:H thin films. In this context, *a*-SiN_x:H thin films were deposited by Hg-sensitized Photo-CVD technique and for the first time the analytical capabilities of Soft X-ray reflectivity technique to obtain depth graded compositional details and growth kinetics of Si-rich *a*-SiN_x:H film is presented and modeled. Additionally, to explore this material for next generation extreme ultraviolet technology, optical constants 'δ' (dispersion) and 'β' (absorption) are evaluated.

Further, combined studies of Elastic Recoil Detection Analysis and X-ray Photoelectron Spectroscopy reveal that less incorporation of hydrogen in ASD *a*-SiN_x:H thin films with moderate Si content favours separation and stabilization of silicon and silicon nitride phases and enable unreacted Si atoms to cluster after Rapid Thermal Annealing (RTA). In addition, under RTA considerable densification and increase in refractive index is noticed due to out-diffusion of hydrogen. The observed phase separation depends upon the stoichiometry of *a*-SiN_x:H thin film rather than the nature of precursor gas. In addition to the above, significant amount of hydrogen entrapment and hydrogen in-diffusion was observed. Further, to understand the thermodynamic stability of the *a*-SiN_x:H/Si structure, conventional furnace annealing has been performed. Similar results in context with the densification of *a*-SiN_x:H thin films were observed upon conventional furnace annealing and attributed to combined effect of hydrogen out-diffusion and structural relaxation. Depending upon the reactant gas flow rate ratio ($R=SiH_4/NH_3$), density of the interfacial layer between *a*-SiN_x:H/Si structure was found to be strongly influenced by annealing. A strong correlation is observed between interface state density and interfacial layer density of the ASD and post-deposition annealed *a*-SiN_x:H thin films.

In addition, optical, physical and structural studies reveal that the phase evolution of as-deposited *a*-SiN_x:H thin films is a function of 'R'. Stoichiometry of ASD *a*-SiN_x:H thin film undergoes a change from *a*-SiO_xN_y:H to Si-rich *a*-SiN_x:H with dominant silicon nitride phase, as 'R' is increased. Hydrogen content was found to be the least in the *a*-SiN_x:H thin film exhibiting silicon phase separation and dominant silicon nitride phase. In addition, red shift in the photoluminescence peak position is observed which is attributed to quantum confinement effect of *in-situ* formed partially crystalline Si-nanostructures in *a*-SiN_x:H matrix. As evidenced by ERDA, the overall phase evolution and *in-situ* formation of Si-nanostructures is dependent on initial hydrogen content, which clearly suggests the involvement of hydrogen in phase separation and partial crystallization of Si-nanostructures.

Finally, investigation were initiated to understand the influence of Swift Heavy Ion (100 MeV Ni^{8+}) irradiation on phase evolution of non-stoichiomtetric *a*-SiN_x:H thin films. The phase composition of *a*-SiN_x:H thin films was found to be dependent on initial hydrogen content. More refined Si network, having dominant Si_3N_4 phase is found to be induced by higher fluence of irradiation. A novel effect of Si-nanostructures dissolution and their re-nucleation upon increase of heavy ion irradiation fluence has been observed and discussed, which offers a new method to synthesize Si-nanostructures of controlled size and uniform distribution in *a*-SiN_x:H matrix.

Currently, I am working as a Research Fellow at National University of Singapore (Singapore) and my research is focus on the 2D transition metal dichalcogenides based electrical devices.

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