ABSTRACT

The outstanding characteristics of hexagonal boron nitride (hBN) layers have recently harnessed significant scientific attention because of their potential applications in electronic and optoelectronic devices. The literature is quite rich in understanding the behaviour of exfoliated hBN films, which find limitations in various emerging applications. Wafer-scale hBN films are potential candidates for practical device applications. However, the unavoidable wrinkles and defects which develop during the growth process, render the characteristics of these films significantly different from their exfoliated counterparts. The thesis discusses a few characteristics of large-scale hBN films of different thicknesses, grown on sapphire substrates, using metal-organic vapour phase epitaxy (MOVPE) technique. Wrinkles lead to strain distribution in the films. Raman imaging is utilized to study the residual strain distribution in the wrinkled hBN films. An increase in the overall compressive strain in the films with an increase in the layer thickness is observed and explained. The study highlights its distribution and origin over the as-grown film area. Next, the thermal response of these as-grown films is explored. The cumulative contributions of anharmonic phonon decay, lattice thermal expansion, defect, and strain modulation due to the change in temperature are considered to investigate the thermal behaviour of the as-grown films. It is revealed that during the heat treatment, the strain evolution due to the differential thermal expansion coefficient of film and substrate plays a dominating role in governing the thermal characteristics of the wrinkled as-grown films. The study is further extended to investigate the interactions of delaminated and transferred large-scale hBN films with different other substrates (SiO_2/Si, sapphire, and quartz). Statistical analysis of the spectral parameters of the Raman mode provides the overall characteristics of the films, which suggests that not only the roughness but also the height modulation at the surface of the substrates play a pivotal role in determining substrate-mediated mechanical strain inhomogeneity in these films. Additionally, it is also found that the slippage of the films during the thermal treatment determines the net strain in the transferred films. Finally, the thermal conductivity of wafer-scale hBN films is determined using Raman spectroscopy, as an optothermal non-contact technique and finite element analysis (FEA). The study decouples the effect of unavoidable wrinkles and defects in determining the thermal conductivity of these hBN films. The crucial role of wrinkles in determining the thermal conductivities of these large-scale films is revealed. Unlike exfoliated films, non-monotonic change in the thermal conductivity with the thickness of wafer-scale hBN films is demonstrated. Utilizing FEA, heat conduction for varying wrinkle densities, suspended geometries, and sizes of circular micro-wells are explored. Though investigated for MOVPE-grown hBN films, the formalisms followed are applicable for any other large-scale 2D materials with defects/wrinkles and grown by other techniques, e.g., CVD or MBE.

Keywords: hexagonal boron nitride, Raman scattering, wrinkle, strain, thermal conductivity