Anharmonic processes and interaction of epitaxial h-BN layers: high temperature Raman spectroscopy studies

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Due to the sp^2 hybridization and a wide band-gap hexagonal boron nitride (h-BN) can substantially contribute to the development of novel optoelectronic devices. In order to fulfill its technological potential, the growth of wafer-scale h-BN of high quality is necessary. This can be achieved by Metal-Organic Vapor Phase Epitaxy (MOVPE) [1]. In this report temperature-dependent Raman spectroscopy studies of epitaxial h-BN grown by MOVPE on sapphire substrates are presented. Raman studies of h-BN available so far in the literature are limited to temperatures up to about 500 K [2] due to defect-related luminescence hindering the observation of the Raman signal. We, however, present data in the temperature range from 300 K up to 1200 K and show that the above-mentioned luminescence can be successfully quenched by annealing samples in a nitrogen atmosphere at temperatures of about 1000 K (Fig. 1.). Our data provides information about the quality of epitaxially grown layers and allows to compare the influence of anharmonic processes [3,4] on thermal properties of bulk h-BN crystals and epi-layers of different thicknesses (Fig. 2.). The obtained energies of the E_{2g}^{high} in-plane phonon mode are slightly higher for epitaxial h-BN as compared to unstrained bulk crystals. This can be explained by strain induced during the growth of epitaxial layers. Interestingly, the temperature induced change of the E_{2g}^{high} energy is similar for bulk material and as-grown epitaxial layers. This is surprising, since, in case of epi-layers, one also deals with the interaction of the h-BN epi-layer with the substrate [5], which originates from their different thermal expansion coefficients. In order to explain this observation, measurements on delaminated epitaxial h-BN films transferred to silicon substrates were performed [6]. They show a large difference compared to the epitaxial layers (Fig. 2.). The obtained data is discussed in terms of different interaction types of the epitaxial layers with the substrate.



1375 1370 1365 1360 ^{high} [cm⁻¹] 1355 1350 bulk + anharmonic ៍_{ត្ត} 1345 ш F178 (~10nm): 1340 h-BN/sapphire h-BN/Si 1335 G032 (~18nm): h-BN/sapphire 1330 h-BN/Si 1325 E 400 600 800 1000 1200 T [K]

Fig. 1. Raman spectra of epitaxial h-BN before and after annealing to 1100K.

Fig. 2. The energy of E_{2g}^{nugn} mode as a function of temperature for h-BN layers.

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- [1] A. K. Dąbrowska et al., 2D Mater. 8, 015017 (2021).
 [2] K. Bera et al., Nanotechnology. 32, 075702 (2021).
- [3] M. Balkanski et al., Phys. Rev. B 28, 1928 (1983).
- [4] R. Cuscó et al., Phys. Rev. B 94, 155435 (2016).

[5] S. Linas et al., Phys. Rev. B **91**, 075426 (2015).

[6] J. Iwańki et al., Acta Phys. Pol. A **139** (2021)