

Temperature induced anomalous vibrational properties of epitaxial boron nitride

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Hexagonal boron nitride (hBN) as an atomically flat, two-dimensional insulator, appears in many novel applications (e.g., van der Waals heterostructures). However, most of the applications are based on small flakes exfoliated from the bulk crystal. In many cases, it is an obstacle which hinders the introduction of hBN in large-scale applications. One possible solution for this problem is epitaxial growth that permits to obtain few-inch area layers [1]. However, the structural and optical quality of epitaxial layer is still inferior to flakes exfoliated from the bulk crystal [2]. Improving the quality of epitaxial layers requires a deeper understanding of the defect properties and their mechanisms of creation.

In this work, we present E_{1u} hBN phonon studies in broad range of temperatures (160-540~K) using Fourier-transform infrared spectroscopy (FTIR). We measured delaminated [3] as well as as-grown epitaxial layers. Here we would like to focus on an anomalous giant shift of phonon energy observed for both types of samples. The phonon energy upshift is correlated with the decrease of spectral peak integral coming from lorentzian fitting as presented in Fig. 1. The temperature for which the anomaly occurs is sensitive to heating, cooling and light irradiation. We present a model involving temperature induced redistribution of the charge on defects what changes their charge state. This in turn causes compressive strain in the epitaxial layer, that would have to be of the order 0.1% to explain the observed shift [4]. The narrow temperature range in which the anomalous behavior takes place raises the question of an involvement of pyro- and piezoelectric effects, which can be expected for non-centrosymmetric stackings of BN monolayers [5].

Acknowledgement: This work was supported by the National Science Centre, Poland, under decisions 2019/33/B/ST5/02766 and 2020/39/D/ST7/02811.

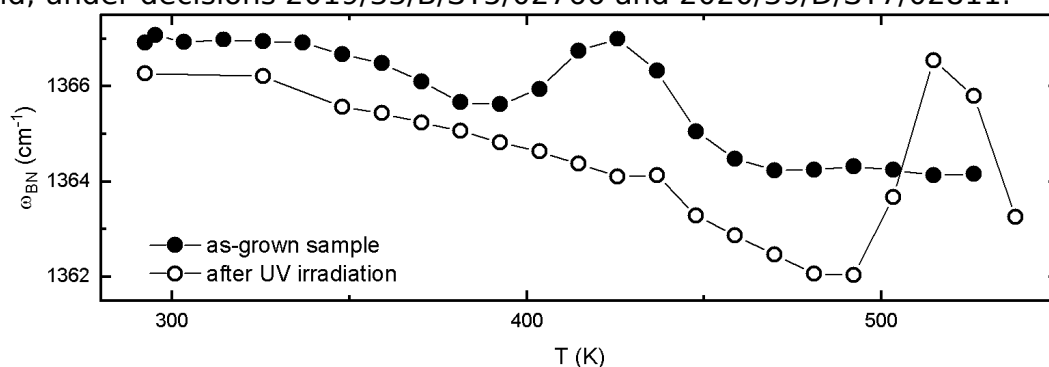


Fig. 1. hBN E_{1u} phonon energy as a function of temperature for as-grown sample (filled circles) and after UV irradiation (opened black circles). The anomalous behavior occurs for ~425 K (for as-grown) and ~520 K (for UV irradiated). Lines are guides to the eyes.

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