

According to the World Health Organization, more than 0,8 million people die each year from diarrhea as a result of unsafe drinking water, sanitation and hand hygiene. Most of these cases could be prevented by proper disinfection. In addition, human development and climate change require even faster progress in sterilization techniques. One of the most effective methods is to use light with a wavelength of about 250 nm. It turns out that such light is very effective in destroying the nucleic acids of microorganisms (such as bacteria, viruses, molds and other pathogens) and disrupting their DNA, leaving them unable to perform vital cellular functions. Therefore, one possible pathway to solve sterilization problems is deep ultraviolet (DUV) light sources (200-280 nm, which corresponds to energies of 4.4-6.2 eV). Unfortunately, the efficiency of semiconductor light sources drops dramatically with decreasing wavelength and in the DUV range is as low as a few percent, which is insufficient for any widely used applications.

In this project, we plan to conduct research on hexagonal boron nitride alloys with aluminum and gallium ($\text{hB}_{1-x-y}\text{Al}_x\text{Ga}_y\text{N}$, x and y correspond to the concentration of Al and Ga, respectively). Hexagonal boron nitride (hBN) has a honeycomb structure with layers stacked on top of each other, analogous to graphite. However, unlike highly conductive graphite, hBN is an insulator with a bandgap about 6 eV which enables light emission in the DUV range. Since the efficiency of light emission, quantum wells are usually used. This requires selecting layers of materials with different bandgaps. In this project, we would like to realize this by the appropriate alloys of hBN with aluminum (Al) and gallium (Ga). Theoretical predictions suggest that adding Al or Ga to hBN should decrease the hBN bandgap. Such a $\text{hB}_{1-x-y}\text{Al}_x\text{Ga}_y\text{N}$ layer could then be placed between the layers of material with a larger bandgap - like pure hBN or hBAlGaN with different concentrations of Al and Ga, creating a quantum well structure.

Although theoretical predictions suggest that quantum wells based on hBAlGaN are feasible, they remain experimentally demanding. Firstly, to grow hBN, we need significantly different conditions than to grow AlN or GaN. Therefore, we will explore the very specific combinations of growth parameters that allow us to obtain alloys with the desired concentration of Al and Ga. Secondly, hBN belongs to the class of two-dimensional materials with a strong covalent bond (sp^2) in the atomic plane and a weak van der Waals bond between subsequent atomic layers. On the other hand, AlN and GaN have a strong sp^3 bond. It is not clear whether the system will tend spontaneously to the sp^3 phase when Al and Ga are added to hBN. And if so, at what concentration of these elements will it occur. Another undiscovered area that we will focus on is how the admixture of Al and Ga will modify the $\text{hB}_{1-x-y}\text{Al}_x\text{Ga}_y\text{N}$ bandgap width and the efficiency of light emission during excitonic transitions. The current knowledge about hBAlGaN mixed crystals is based mainly on simulations and has not been confirmed experimentally. That is why in this project we will try to experimentally verify the correctness of theoretical calculations. Our initial results show that we are able to alloy hBN with Ga which affects the absorption coefficient as well as width of the bandgap while maintaining the sp^2 layered structure.

To answer the above questions, we plan to conduct systematic studies on hBAlGaN samples grown by us on two-inch sapphire substrates using metalorganic vapor phase epitaxy (MOVPE). Then we will characterize them comprehensively using spectroscopic (UV-Vis spectroscopy, Raman spectroscopy, Fourier-transform infrared spectroscopy, photoluminescence), X-ray (X-ray diffraction, X-ray photoelectron spectrometry, energy-dispersive X-ray spectroscopy) and electron microscopy (scanning electron microscopy, transmission electron microscopy) methods. The experiments conducted will allow us to draw conclusions about the dependence of the width of the bandgap and, in particular, about the possibility of changing the nature of the bandgap from indirect to direct, which would result in enhanced DUV emission efficiency. We will also optimize the hBAlGaN mixed crystal growth process to obtain good quality material with a boron concentration of 90-100%. Our studies will lead to a better understanding of how to effectively alloy hBN with Al and Ga, and will provide insights into the relationship between the hBAlGaN composition and its electronic structure, including mixing of the indirect-direct nature of the bandgap. This aspect is very interesting in terms of comprehension the basic properties of hBAlGaN mixed crystals and from the point of view of future DUV optoelectronic applications such as efficient light sources enabling efficient sterilization.