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Boron phosphide grown by PECVD and its optical properties

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Abstract. This article presents a study of the growth of boron phosphide (BP) thin films by plasma enhanced chemical vapor deposition (PECVD) and its optical properties. BP thin films were deposited on a fused silica and silicon substrates using a mixture of diborane (B_2H_6) and phosphine (PH_3) with hydrogen as precursors. The optical properties were investigated using optical spectroscopy, which showed excellent optical transparency in the visible and near-infrared regions. The BP films exhibited a bandgap of approximately 1.9 eV, indicating its potential for use in optoelectronic applications. The results demonstrate that PECVD is a promising technique for growing BP thin films with desirable optical properties.

Keywords: boron phosphide, PECVD, plasma enhanced chemical vapor deposition, optical spectroscopy

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Плазмохимическое осаждение фосфида бора и его оптические свойства

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Аннотация. В этой статье представлено исследование роста тонких пленок фосфида бора (BP) методом плазмохимического осаждения и его оптических свойств. Тонкие пленки BP осаждались на кварцевую подложку с использованием смеси диборана

(B_2H_6) и фосфина (PH_3) с водородом в качестве прекурсоров. Оптические свойства были исследованы с помощью оптической спектроскопии, которая показала высокую оптическую прозрачность в видимой и ближней инфракрасной областях. Пленки BP имели ширину запрещенной зоны примерно 1,9 эВ, что указывает на их потенциал для использования в производстве оптоэлектронных приборов. Результаты показывают, что плазмохимическое осаждение является многообещающим методом выращивания тонких пленок BP с требуемыми оптическими свойствами.

Ключевые слова: фосфид бора, плазмохимическое осаждение, оптическая спектроскопия

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Introduction

Boron phosphide (BP) is a novel material for use in photovoltaics that has a number of attractive characteristics. BP is chemically inert, resistant to oxidation at high temperatures, has high thermal conductivity, low toxicity and mechanical stability [1]. It has also been theoretically shown that BP is one of the most promising materials for creating transparent conductive p-type coatings, since it is an indirect-gap semiconductor with a band gap of 2.1 eV, while the band gap for a direct transition is 4 eV, which implies low optical losses [2].

Due to these properties, the use of boron phosphide to create solar cells can increase the short circuit current compared to the use of amorphous hydrogenated silicon (a-Si:H). On the other hand, the negative (−0.3 ± 0.1 eV) valence band gap offset (ΔE_V) for the BP/Si interface [3] provides the necessary selectivity, which makes boron phosphide an excellent candidate for a selective hole contact without requiring an additional indium tin oxide layer (ITO) [4].

One of the key challenges in producing high-quality BP thin films is the availability of a suitable deposition technique. Among the various deposition methods, plasma-enhanced chemical vapor deposition (PECVD) has emerged as a promising technique for growing BP thin films due to its advantages such as scalability, low deposition temperatures, cost-effectiveness, and compatibility with large-area substrates.

In this article, we present a study on the growth of BP thin films by PECVD and their optical properties. The optical properties of BP thin films are critical to their performance in optoelectronic devices. Therefore, their characterization is essential for assessing their potential applications in energy-related fields. The results of this study provide valuable insights into the use of PECVD as a method for growing BP thin films with desired optical properties, which could facilitate its integration into various optoelectronics applications.

Materials and Methods

The growth of BP films was carried out in a standard Oxford PlasmaLab 100 PECVD (13.56 MHz) plasma chemical deposition unit using capacitive coupled RF plasma with a precursors flow control and temperature control of a heating table. Gas mixtures of 100 sccm hydrogen with 20 sccm of diborane (B_2H_6) and 10 sccm of phosphine were used as precursors. BP layers were deposited on fused silica and silicon substrates with orientation (100) at a low temperature (350 °C). The deposition was carried out at a plasma power of 100 W for 30 minutes with 600 mTorr chamber pressure.

Structural properties and surface morphology of the BP layer deposited on the silicon substrate was studied by means of transmission electron microscopy (TEM) using Jeol JEM-2100F set-up with 200 kV acceleration voltage (point resolution 0.19 nm). Cross-section specimens for TEM were prepared by conventional route involving mechanical grinding with subsequent ion milling by Ar^{+} at 2–4 kV. Energy dispersive X-ray spectroscopy (EDX) and electron energy loss spectroscopy (EELS) implemented in the TEM were used for the BP layers composition evaluation.

Optical transmission and reflection spectra were obtained on BP film deposited on fused silica substrates with Avantes ULS2048 spectrometer and Xe light source. Optical band gap parameters for BP thin layers were evaluated by a Tauc plot for indirect band gap semiconductors [5].

Results and Discussion

Fig. 1 shows Electron Energy Loss Spectra (EELS) and Transmission Electron Microscopy (TEM) image of the BP film on silicon substrate. According to EELS layer has semi-stoichiometric composition of elements with ratio of 60% of boron and 40% of phosphorus. TEM images of BP sample (Fig. 1) demonstrate the amorphous structure the film compared to the clearly distinguishable crystalline state of the Si substrate. The BP layer has a smooth surface and homogeneous structure with lack of visible defects. Heterointerfaces between Si substrate and BP layer are sharp and smooth. No initial epitaxy or any intermediate layer are observed.

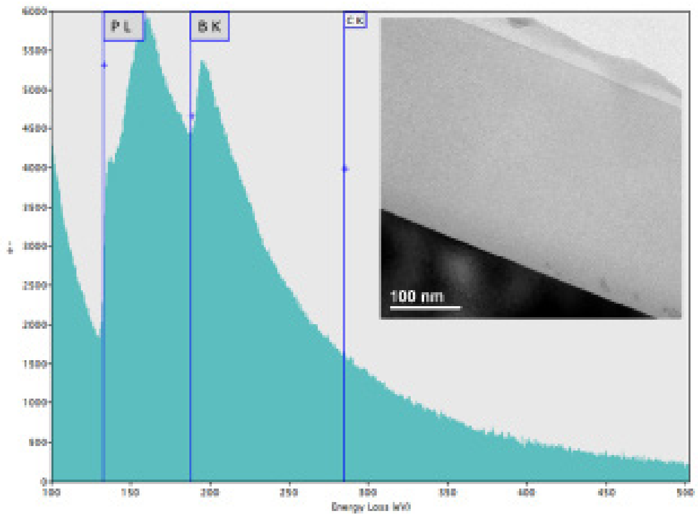

Fig. 1. Electron Energy Loss Spectra (EELS) and
Transmission Electron Microscopy (TEM) image of the BP film

Fig. 2,*a* shows absorbance spectra, boron phosphide is quite transparent in the long wavelength region (from 600-1100 nm), while in the short-wavelength region absorbance increases.

Fig. 2,*b* shows the Tauc plot for indirect bandgap, in which the gap value can be extracted. The gap value for the BP layer is 1.93 eV, which is in agreement with literature data. According to [3], the band gap for a-BP:H is in the range of 2.0–2.1 eV and depends on both the hydrogen and phosphorus proportion. The layer thickness was determined, the value of which is about 300 nm.

Table 1

Deposition properties

Temperature, °C	Deposition time, min	Pressure, mTorr	Plasma power, W	Growth rate, nm/min	$B_2H_6/PH_3/H_2$, sccm
350	30	600	100	12.3	20/10/100

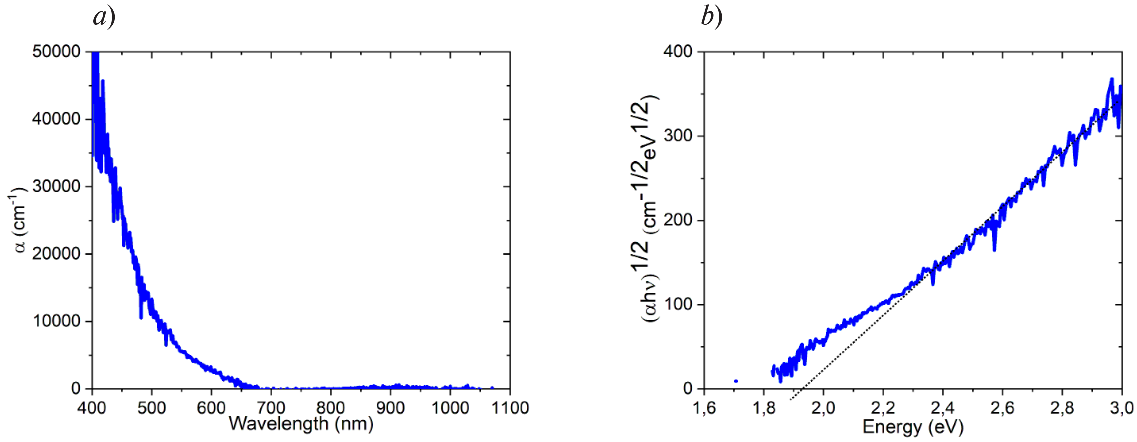

Fig. 2. Absorbance specter of BP film (*a*), Tauc plot for the indirect bandgap (*b*)

Conclusion

Thus, for the first time, boron phosphide was successfully deposited at low temperature (350 °C) by the plasma enhanced chemical vapor deposition (PECVD) method and its optical properties were studied. Film demonstrated high transparence in a long wavelength range and its band gap value extracted from the Tauc plot is in a good agreement with the literature.

This study provides a valuable contribution to the field of materials science, as BP is a promising material for various optoelectronic and photovoltaic-related applications. The use of PECVD as a deposition technique facilitates the integration of BP thin films into various device architectures, as it is scalable, cost-effective, and compatible with large-area substrates. Further research can leverage the results of this study to optimize the deposition process of BP by PECVD and explore its potential applications in optoelectronics, photovoltaics, and catalysis. Furthermore, the electronic properties of BP needs to be investigated.

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