



# Spatial solitons supported by graphene/hexagonal boron nitride heterostructures

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## ABSTRACT

In this paper, we show how the diffraction of light beams is balanced by the nonlinearity of graphene/hexagonal boron nitride heterostructures, which discretely occurs in the very thin graphene layers, forming spatial solitons. We also discuss the effects of the layer number and the peak *E*-field amplitude on the soliton width.

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## 1. Introduction

Two-dimensional (2D) materials have attracted great research interest since the first isolation of graphene [1]. The properties of these materials are usually very different from those of their 3D counterparts [2]. With these properties, 2D materials offer a good platform to create heterostructures, a combination of several 2D materials in one vertical stack by van der Waals forces [3]. As the family of 2D crystals is expanding day by day, such heterostructures allow a far greater number of combinations, which lead to the observation of numerous exciting physical phenomena [4,5]. Among various heterostructures, the combinations of graphene with hexagonal boron nitride (hBN), especially the one that hBN is sandwiched between graphene layers, are particularly attractive, because of the unique crystalline quality and the small lattice mismatch of them [6,7]. For example, it was reported that a twist-controlled resonant tunnelling can be achieved in graphene/boron nitride/graphene heterostructures [8], and it was shown possible to increase the oscillation frequency of graphene resonant tunneling diodes by utilizing hBN [9].

On the other hand, nonlinearity exists naturally in many optical systems, which profoundly affects the propagation of light. Among others, one of the nonlinear effects with great potential is the

formation of optical solitons, including temporal and spatial solitons [10]. Previous studies have shown that graphene is a Kerr nonlinear medium with a very large third-order nonlinear optical susceptibility, which was theoretically reported [11,12] and experimentally verified [13].

## 2. Materials and methods

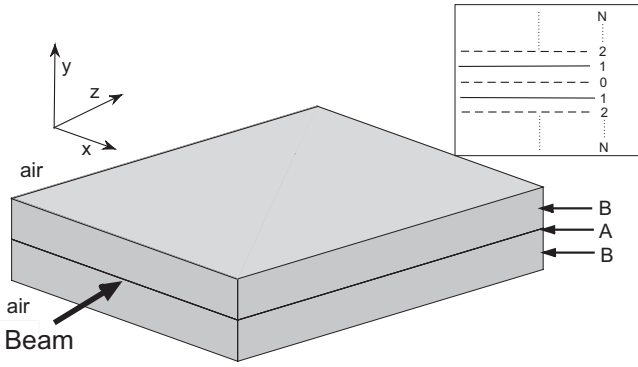
The structure in our analysis is shown in Fig. 1. A heterostructure which consists of alternately arranged graphene and hBN layers is placed inside a planar  $\text{SiO}_2$  waveguide, outside of which is air. At the center of the heterostructure, there is a hBN layer, labeled as '0'. There are two layers of graphene on both sides (above and below) of '0' layer, labeled as '1'. Then there are two layers of hBN on both sides (above and below) of '1' layers, labeled as '2'... and so on, until the layers labeled as 'N'.

To account for the formation of spatial solitons, we start with the theoretical approach used to describe soliton formation in conventional 3D nonlinear media. Within this approach the propagation of an optical beam in a Kerr nonlinear medium is governed by the  $(2+1)$ -dimensional nonlinear Schrödinger (NLS) equation [10,14,15]

$$2i\beta \frac{\partial \Phi}{\partial z} + \left( \frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} \right) + 2\beta^2 \frac{n_2}{n_0} |\Phi|^2 \Phi = 0, \quad (1)$$

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**Fig. 1.** Schematic diagram of a heterostructure (A) sandwiched between two 150 nm SiO<sub>2</sub> layers (B). Such a structure is surrounded by air. The inset shows the components of the heterostructure, which is formed by alternately arranged graphene (solid lines) and hBN (dashed lines) layers.

where  $\Phi = \Phi(x, y, z)$  is the envelope of the electric field,  $\beta = k_0 n_0 = 2\pi n_0 / \lambda_0$ , and  $n_2 = 3\chi^{(3)} / 8n_0$ . If the field in the  $y$ -direction is defined by the guided mode of the slab waveguide [16], one can obtain a solution in the form of a canonical first-order soliton in the  $x$ - $z$  plane

$$E(x, z) = \frac{\lambda_0}{\pi a_0} \sqrt{\frac{2}{3\chi^{(3)}}} \exp\left(\frac{i\lambda_0 z}{4\pi n_0 a_0^2}\right) \operatorname{sech}\left(\frac{x - x_0}{a_0}\right), \quad (2)$$

where  $a_0$  is a measure of the soliton width.

We now come back to consider our problem. Since the third-order nonlinear optical susceptibility of graphene is several orders of magnitude larger than that of hBN and SiO<sub>2</sub>, we neglect the nonlinear effects of hBN and SiO<sub>2</sub>. As the thickness of monolayer is much smaller than the wavelength, the structure can be modeled by a homogeneous one, where the position-dependent properties are replaced by homogeneous parameters. Here we employ  $\bar{n}_0$  and  $\bar{\chi}^{(3)}$  as the homogeneous parameters to represent the linear refractive index and the third-order nonlinear susceptibility respectively. The calculated values of the homogeneous parameters corresponding to different layer numbers are listed in Table 1, where  $h$  represents the thickness of the homogeneous heterostructure. Throughout this paper, the operating wavelength considered is  $\lambda_0 = 850$  nm. In the calculation, we take the third-order nonlinear susceptibility of graphene directly from the experiment as  $\chi^{(3)} = 2.095 \times 10^{-15} \text{ m}^2/\text{V}^2$  [13], approximate the thickness of monolayer of graphene and hBN by  $d_0 = 0.3$  nm, and take the values of the linear refractive indexes of graphene and hBN to be  $n_{01} = 3.0$  and  $n_{02} = 2.2$  respectively.

So far, we have homogenized the heterostructure and obtained a set of homogeneous parameters. However, there are two layers of SiO<sub>2</sub> on both sides as well as the air outside which need to be considered. Actually, the linear refractive index and nonlinear refractive index that the beam “sees” are the effective ones, so we need to further calculate the equivalent values of them, which can be obtained based on the energy distributions of the electromagnetic (EM) modes in different media [17].

**Table 1**  
Values of the homogeneous parameters of the heterostructure.

$N$	1	2	3	4	5	6	7	8
$\bar{n}_0$	2.73	2.52	2.66	2.56	2.64	2.57	2.63	2.58
$\bar{\chi}^{(3)}$	1.397	0.838	1.197	0.931	1.143	0.967	1.117	0.986
$h$	0.9	1.5	2.1	2.7	3.3	3.9	4.5	5.1

The units of  $\bar{\chi}^{(3)}$  are  $10^{-15} \text{ m}^2/\text{V}^2$  and the units of  $h$  are nm.

Taking the above arguments into consideration, the soliton solution to Eq. (2) becomes

$$E(x, z) = \frac{\lambda_0}{\pi a_0} \sqrt{\frac{2}{3\chi_{(equ)}^{(3)}}} \exp\left(\frac{i\lambda_0 z}{4\pi n_{0(equ)} a_0^2}\right) \operatorname{sech}\left(\frac{x - x_0}{a_0}\right), \quad (3)$$

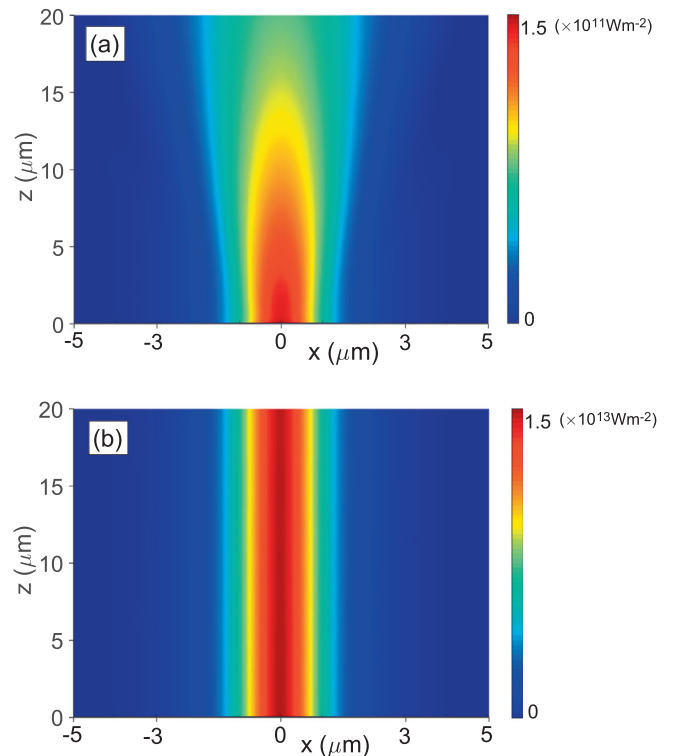
where the subscript (*equ*) represents the corresponding equivalent value.

### 3. Results and discussion

We next investigate the soliton formation and its properties using the software package FDTD Solutions and Mode Solutions [18].

As an example, we first demonstrate the soliton formation for the layer number  $N = 3$ . The incident beam is  $E_x$ -polarized propagating along the  $z$ -direction with a sech shape in the  $x$ -direction and a waveguide profile in the  $y$ -direction. Fig. 2 illustrates the formation of a spatial soliton at the operating wavelength  $\lambda_0 = 850$  nm, which remains unchanged throughout this paper. Unlike the soliton formation in conventional media, here in our system, the nonlinearity only occurs in the very thin graphene layers, discrete along  $y$ -direction.

We next investigate the dependence of the soliton width (characterized by  $a$ ) on the layer number (characterized by  $N$ ) of the heterostructure. We have computed the soliton profiles for  $N = 1-8$  with the same peak  $E$ -field amplitude, i.e.,  $|E|_{\max} = 6.5 \times 10^7 \text{ V/m}$ . The results are summarized in Fig. 3a, where the values of the soliton width (star points) are obtained at the central linear hBN layer by fitting the  $E$ -fields with sech functions. As shown in Fig. 3a, the soliton width changes obviously when  $N$  changes from even to odd, but when  $N$  changes from odd to even, it changes little. The reason is that when  $N$  changes from even to odd, two graphene layers with large nonlinearity are added



**Fig. 2.** Intensity of a propagating beam evaluated at the central linear hBN layer (labeled as ‘0’) for the low intensity regime (a) and the soliton (high intensity) case (b).

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