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Peculiarities of the propagation of multidimensional extremely short optical pulses in germanene

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ABSTRACT

In this Letter, we study the propagation characteristics of both two-dimensional and three-dimensional extremely short optical pulses in germanene. A distinguishing feature of germanene—in comparison with other graphene-like structures—is the presence of a significant spin–orbit interaction. The account of this interaction has a significant impact on the evolution of extremely short pulses in such systems. Specifically, extremely short optical pulses, consisting of two electric field oscillations, cause the appearance of a tail associated with the excitation of nonlinear waves. Due to the large spin–orbit interaction in germanene, this tail behind the main pulse is much smaller in germanene-based samples as compared to graphene-based ones, thereby making germanene a preferred material for the stable propagation of pulses along the sample.

1. Introduction

In recent years, graphene-like structures have generated increased attention from researchers interested in the nonlinear propagation of light in two-dimensional structures, which—because of the reduced dimension—have unique properties valuable in modern micro- and nanoelectronics [1]. Such materials include, for example, silicene, consisting of a single layer of silicon atoms in a hexagonal lattice [2,3]. A distinctive feature of the silicene is a significantly stronger spin–orbit interaction in comparison to graphene. In recent studies, the authors investigated the propagation of extremely short one-dimensional electromagnetic pulses in silicene waveguides [4]. One of the most interesting predictions for it is the existence of the band gap, which can lead to the appearance of a transition between the itinerant and the topological insulator. In turn, the emergence of the band gap in the electronic spectrum has a significant impact on the dynamics of multidimensional extremely short optical pulses. Furthermore, it is important noting that the magnitude of the band gap is largely determined by the spin–orbit interaction. Hence, identifying two-dimensional structures with stronger spin–orbit interaction offers promising prospects for the development of new materials for the optoelectronics industry. At the same time, one shall not ignore the fact that silicon still remains the primary constituting element of modern microelectronics devices.

In search for such new materials and structures, the germanene was proposed. Essentially, it is a two-dimensional material with a hexagonal lattice, similar to silicene, but manufactured on the basis of germanium as opposed to using classical silicon [5,6]. Recent results show that the spin–orbit interaction for germanene is more than 10 times larger than that of silicene, and thus 10,000 times larger than for graphene [7]. This leads to a significant increase in the size of the band gap in the spectrum, which in turn leads to a change in the dynamics of the propagation extremely short pulses of light in such an environment. This Letter is specifically aimed at studying this latter point.

2. Fundamental equations

In the long-wavelength approximation, the Hamiltonian for germanene can be written as [7,8]:

$$H = v\left(\xi p_x \sigma_x + p_y \sigma_y\right) - \frac{1}{2}\xi \Delta_{SO} \tau_z \sigma_z + \frac{1}{2}\Delta_z \sigma_z, \tag{1}$$

where $v = 4.6 \times 10^5$ m/s is the velocity of Dirac electrons, $\xi = \pm 1$ is the valley sign for two Dirac points, $\mathbf{p} = \{p_x, p_y\}$ is the electron quasi-momentum, $\Delta_{SO} = 43$ meV is the strength of the spin–orbit interaction in germanene ($\Delta_{SO} = E_{0z} d$), E_{0z} is the constant electric field, d is distance between the two sublattice planes, Δ_z is

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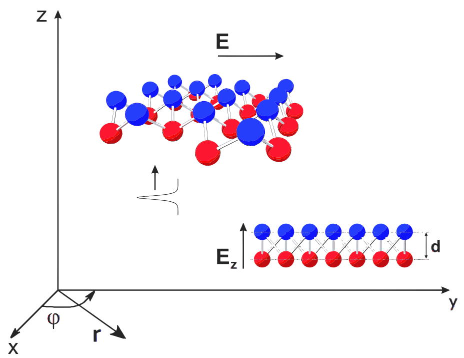

Fig. 1. Geometry of the problem.

the spectrum band gap, σ_i and τ_i are the Pauli matrices [9]. The geometry of the problem is illustrated by the schematic diagram in Fig. 1.

Writing the Hamiltonian in a matrix form, it is easy to obtain the spectrum of electrons:

$$\varepsilon_{\sigma\xi} = \pm\sqrt{v^2k^2 + \frac{1}{4}(\Delta_z - \sigma\xi\Delta_{SO})^2}, \tag{2}$$

where σ stands for the electron spin. Using similar arguments as in Ref. [4], we can write the governing equation for the propagation of ultrashort pulses as follows:

$$\frac{\partial^2 \mathbf{A}}{\partial x^2} + \frac{\partial^2 \mathbf{A}}{\partial z^2} - \frac{1}{c}\frac{\partial^2 \mathbf{A}}{\partial t^2} + \frac{4\pi}{c} j(\mathbf{A}) = 0. \tag{3}$$

Here $j(\mathbf{A})$ is determined by finding the density of electric current:

$$j = e\int_{-\Theta}^{\Theta}\int_{-\Theta}^{\Theta} dp_x dp_y v_y \left(\mathbf{p} - \frac{e}{c}\mathbf{A}(x,t)\right), \tag{4}$$

where $v_y(p) = \partial\varepsilon(p_x, p_y)/\partial p_y$. The electric field $\mathbf{E}$ is directed along the z-axis and is considered in the frame of the canonical gauge $\mathbf{E} = -\frac{1}{c}\partial\mathbf{A}/\partial t$. The region of integration over the momenta in Eq. (4) can be determined from the conservation condition for the number of particles:

$$\int_{-\Theta}^{\Theta}\int_{-\Theta}^{\Theta} dp_x dp_y = \iint_{BZ} dp_x dp_y \langle a^{\dagger}_{p_x p_y} a_{p_x p_y}\rangle,$$

where $a^{\dagger}_{p_x p_y}$ and $a_{p_x p_y}$ are creation and annihilation operators of electrons respectively, with quasi-momentum p; the integration in the right-hand-side term is taken over the Brillouin zone (BZ).

In three dimensions, Eq. (3) is recast using the cylindrical coordinates system, and thereby takes the following form:

$$\frac{\partial^2 \mathbf{A}}{\partial t^2} = \frac{1}{r}\frac{\partial}{\partial t}\left(r\frac{\partial \mathbf{A}}{\partial r}\right) + \frac{\partial^2 \mathbf{A}}{\partial z^2} + \frac{1}{r^2}\frac{\partial^2 \mathbf{A}}{\partial \theta^2} + 4\pi j(\mathbf{A}). \tag{5}$$

Assuming that the system is axisymmetric, we have $\partial \bullet /\partial\theta \to 0$. Due to the field inhomogeneity along a certain axis, the resulting current is inhomogeneous, thereby leading to a charge accumulation in some areas. From the charge conservation law, one can conclude that the duration of the ultra-short pulse will have a significant impact on the accumulated charge. Our estimations—the stored charge being about 1–2% of the charge contributing to the

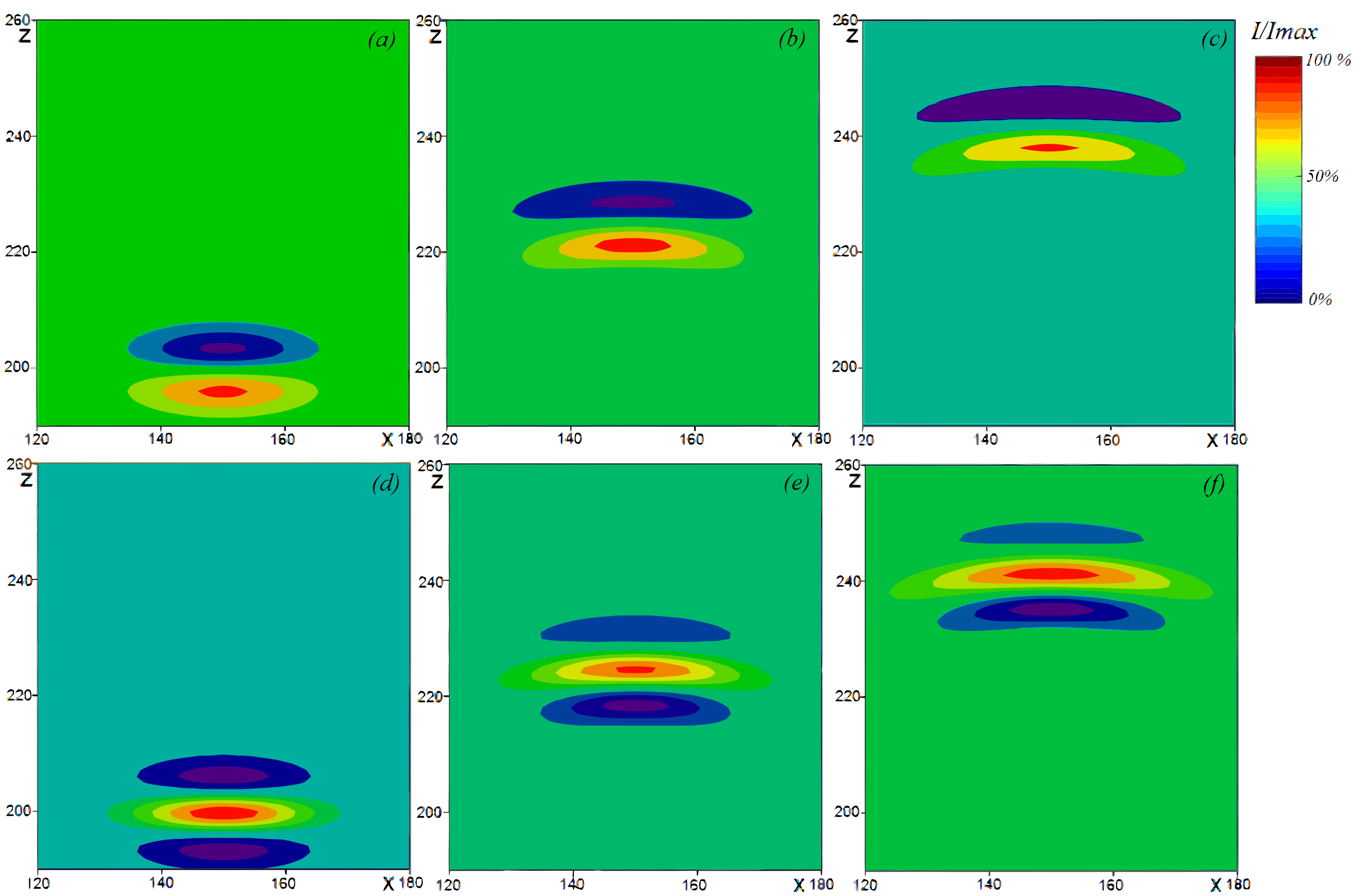

Fig. 2. The intensity of a two-dimensional electromagnetic pulse $I(x,z,t) = E^2(x,z,t)$ consisting of a single (a, b, c) and double (d, e, f) oscillations of electric field at different instances of time: (a, d) – initial pulse; (b, e) – $t = 3\times10^{-13}$ s; (c, f) – $t = 5\times10^{-13}$ s. The unit distance on the axes x and z corresponds to 15 nm.

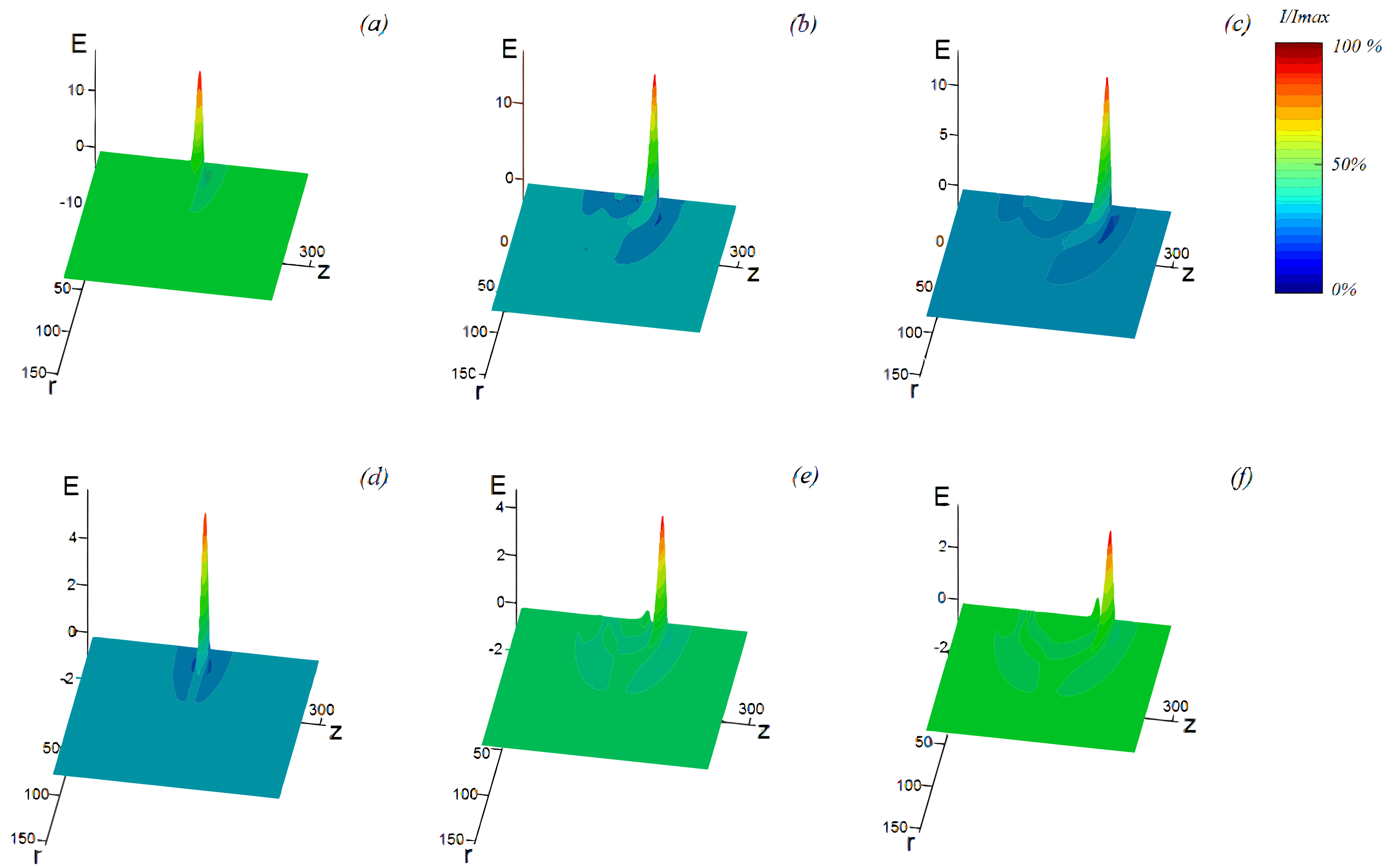

Fig. 3. The intensity of a three-dimensional electromagnetic pulse $I(x,z,t) = E^2(x,z,t)$ consisting of a single (a, b, c) and double (d, e, f) oscillations of electric field at different instances of time: (a, d) – initial pulse; (b, e) – $t = 3 \times 10^{-13}$ s; (c, f) – $t = 5 \times 10^{-13}$ s. The unit distance on the axes r and z corresponds to 15 nm. The electric field E is scaled in 10^7 V/m.

current—suggest that the charge accumulation effect for femtosecond pulses can be ignored [10].

3. Results and discussion

Equations (3) and (5) are solved numerically using classical numerical schemes detailed in Ref. [11]. The initial condition in the two-dimensional case was chosen as a very short pulse, consisting of one oscillation ($n = 0$) and two oscillations ($n = 1$), which can be expressed as follows:

$$A(z,t=0) = Q\, z^n \exp\left(-z^2/\gamma_z\right) \exp\left(-x^2/\gamma_x\right), \tag{6}$$

$$\frac{dA}{dt}(z,t=0) = \frac{2z^{n+1} v_z}{\gamma_z} Q\, z^n \exp\left(-z^2/\gamma_z\right) \exp\left(-x^2/\gamma_x\right). \tag{7}$$

Here Q is the pulse amplitude, v_z is its initial velocity in z-direction, $\gamma_{x,z}$ determine the half-width of the pulse in the x- and z-direction respectively. Time has been chosen as an evolution coordinate.

The initial condition in three dimensions was also selected in two forms—the pulse, consisting of one oscillation ($n = 0$) and two oscillations ($n = 1$):

$$A(z,r,t=0) = Q\,(z-z_0)^n \exp\left(-(z-z_0)^2/\gamma_z\right) \exp\left(-r^2/\gamma_r\right),$$

$$\frac{dA}{dt}(z,r,t=0) = 2Q\,\frac{(z-z_0)^{n+1} v_z}{\gamma_z} \exp\left(-(z-z_0)^2/\gamma_z\right) \times \exp\left(-r^2/\gamma_r\right), \tag{8}$$

where r is the radial coordinate, γ_r is the corresponding half-width along this radial direction, z_0 is the initial displacement of the center of the pulse. This initial condition corresponds to the irradiation of the sample by an extremely short pulse consisting of a single oscillation of the electric field. The values of energy parameters are expressed in units of Δ. Note that, like in the 2D case, time is chosen as an evolution variable.

The resulting evolution of a two-dimensional electromagnetic field propagating in germanene is shown in Fig. 2. The number of electric field fluctuations has a significant impact on the shape of extremely short optical pulse. It can be seen, however, that in the case of both one and two oscillations electric field pulse propagates stably, without the formation of any "tails" behind it. Such a behavior on the one hand is due to dispersion, which leads to a broadening of the optical pulse, and on the other, due to the nonlinear effects—nonlinear terms are apparent in Eq. (3)—which determines its "narrowing". Thus, a stable pulse propagation is possible due to the balance between these two superimposing processes in germanene.

The resulting evolution of the three-dimensional electromagnetic field as it propagates along the sample is shown in Fig. 3. In the case of the zero area pulse, the main pulse comes with the "tail", which speaks in favor of the single field oscillation to ensure the stability of its distribution.

Comparison of the cases of strong versus weak spin–orbit interaction is presented in Fig. 4. As can be seen in Fig. 4, an increase in the parameter Δ_{SO}—parameter that determines the magnitude of the spin–orbit interaction—leads to the formation of a much smaller "tail" behind the main pulse, that is, has a stabilizing effect on the propagation of the pulse. Thus, germanene is a preferred material for the stable propagation of pulses along the sample due to its large spin–orbit interaction.

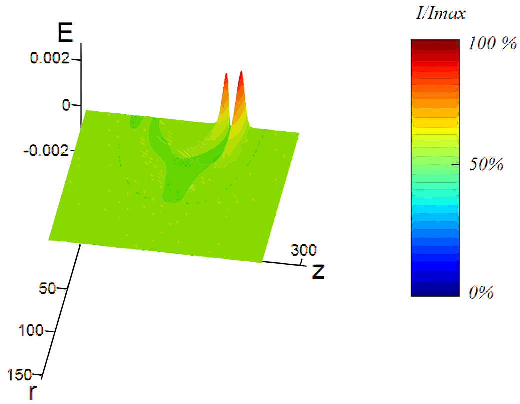

Fig. 4. The difference between the amplitudes of the three-dimensional electromagnetic pulse, consisting of two oscillations of the electric field for germanene ($\Delta_{SO} = 43$ meV) and silicene ($\Delta_{SO} = 3.9$ meV) at time $t = 5 \times 10^{-13}$ s. The unit distance on the axes r and z corresponds to 15 nm. The electric field E is scaled in 10^7 V/m.

In spite of the well established stability properties of germanene (see e.g. Ref. [5] and references therein), the natural question arises if the germanene sample remains stable during the laser pulse propagation. However, this problem is not particularly relevant in our case. The pulse we consider is ultra-short (of a few field oscillations), and the induced current is ballistic. Therefore, the energy is not absorbed by the sample during the propagation event. The long-time relaxation will apparently lead to some energy absorption, but that is a different problem. The object of this current study is the ultra-short pulse itself.

4. Conclusions

Key results of this work may be summarized as follows:

i) The effective equation describing the dynamics of multidimensional extremely short optical pulses in germanene have been established.
ii) The amplitude of extremely short optical pulses does not decay, thereby indicating a certain level of balance between dispersive effects and nonlinear ones for this system.
iii) The effect of the spin–orbit interaction in the process of propagation of extremely short pulses has been account for and demonstrated.
iv) Extremely short optical pulses, consisting of two electric field oscillations, cause the appearance of a “tail” that can be associated with the excitation of nonlinear waves.

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