Solid State Communications 350 (2022) 114774

Contents lists available at ScienceDirect

Solid State Communications

journal homepage: www.elsevier.com/locate/ssc

Communication

Circularly-polarized-pulse-driven ultrafast optical currents in monolayer hexagonal Boron Nitride (*h*-BN)

Prabath Hewageegana [a,*], Vadym Apalkov [b]

[a] Department of Physics, University of Kelaniya, Kelaniya 11600, Sri Lanka
[b] Center for Nano-Optics (CeNO) and Department of Physics and Astronomy, Georgia State University, Atlanta, GA 30303, USA

ARTICLE INFO

Communicated by Xu Wen

Keywords:
Ultrafast optics
Hexagonal Boron Nitride
Topological resonance
Optical currents
Transferred charge

ABSTRACT

We predict the fundamentally fastest, ultrafast optical currents in monolayer hexagonal Boron Nitride (*h*-BN) by a circularly-polarized single-oscillation optical pulse. The femtosecond currents in gapped graphene and transition metal dichalcogenides have been discussed. However, the extension of the gapped graphene model for the large bandgap (~5 eV) has not been shown before. The strong optical pulse redistributes electrons between the bands and generates femtosecond currents during the pulse. The pulse generates both $x-$direction and $y-$direction currents due to charge transfer through the system. Thus, femtosecond ultrashort laser pulses provide an effective tool to manipulate and study the transport properties of electron systems and enhance the conductivity in solids at an ultrafast time scale with high temporal resolution. Ultrafast currents and charge transfer in monolayer *h*-BN may provide a fundamental basis for petahertz-band information processing.

1. Introduction

Femtosecond and attosecond-long ultrashort laser pulses provide an effective tool to manipulate and study the electron dynamics in solids at an ultrafast time scale with a high temporal resolution [1–16]. In particular, two dimensional (2D) materials exhibit unique properties due to the 2D nature of electron dynamics [17]. Among such 2D materials are dichalcogenides, complex oxides, bismuth telluride atomic quintuples, and boron nitride [18,19]. This new world of two-dimensional crystals is still very little researched, both in terms of their fundamental properties and their potential applications [20].

Two-dimensional monolayer hexagonal Boron Nitride (*h*-BN) possesses a direct bandgap of 4–6 eV at the Brillouin zone corner points, K, K' [21–23]. Similar to graphene, *h*-BN has a hexagonal lattice made of two sublattices, A and B (see Fig. 1(a)). Sublattices A and B consist of Boron and Nitride atoms and break the inversion ($\mathcal{P}$) symmetry and opens up gaps at the K, K'-points marking *h*-BN a wide-gap semiconductor [21] with D_{3h} point symmetry group [24,25]. However, the energy-dispersion symmetry between the K and K' valleys is protected by the time-reversal ($\mathcal{T}$) symmetry. Due to the broken inversion symmetry, the Berry curvature (topological magnetic field), $\boldsymbol{\Omega}$, has finite values with opposite signs in two valleys, K, and K', (see Fig. 1(b)). In contrast, the corresponding Berry curvature in graphene is non-zero only at the Dirac points, at which it has a δ-type singularity. The finite Berry curvature gives rise to a new effect, *topological resonance*, which occurs when the electron wave functions gradually accumulate the topological (geometric) phases along the electron Bloch trajectory in the field of the pulse [2–4,12,26]. In monolayer *h*-BN the corresponding Berry curvature is extended over finite regions near the K and K' points (see Fig. 1(b)). This allows electron wave functions, in monolayer *h*-BN, to gradually accumulate the topological phase.

Previously, we have shown that a single cycle of a circularly polarized optical pulse induces a large valley polarization, 25%–50%, in hexagonal Boron Nitride (*h*-BN) monolayers [27]. Such a strong pulse redistributes electrons between the bands and generates a valley-selective conduction band population. The mechanism of producing the fastest valley polarization fundamentally in *h*-BN monolayer has a topological origin [27]. Intense optical pulse contributes to the generation of strong nonlinear electric currents and finite electric charge transfer through the system. This is due to the strong coupling between the valence band (VB) and conduction band (CB) states. VB to CB transitions occur when an electron passes in the vicinity of the Dirac point (K or K') where the interband transition dipole matrix element (non-Abelian Berry connection) is enhanced [2–4].

The femtosecond currents, driven by a linearly-polarized single-oscillation of an intensive laser pulse in gapped graphene [15], and in transition metal dichalcogenides (TMDC) [28] have been discussed recently. However, the extension of the gapped graphene model for the bandgap of *h*-BN has not been shown before. Here, a large bandgap resembling the electronic structure of monolayer *h*-BN is introduced

* Corresponding author.
E-mail address: prabath@kln.ac.lk (P. Hewageegana).

https://doi.org/10.1016/j.ssc.2022.114774
Received 8 August 2021; Received in revised form 15 March 2022; Accepted 17 March 2022
Available online 18 April 2022