Computational Materials Science 155 (2018) 63–68

Contents lists available at ScienceDirect

Computational Materials Science

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

# Electron-phonon investigation in stanene

N.B.-J. Kanga[a,*], S. Insad[a], L.B. Drissi[a,b]

[a] LPHE, Modeling & Simulations, Faculty of Science, Mohammed V University in Rabat, Morocco
[b] CPM, Centre of Physics and Mathematics, Faculty of Science, Mohammed V University in Rabat, Morocco

ARTICLE INFO

*Keywords:*
Stanene
Topological insulator
Hot carriers
Electron-phonon
Linewidth
Scattering rate

ABSTRACT

Collecting carriers before they thermalize is the main goal for carrier's cells. This work presents a study on hot carriers in stanene using density functional and many-body perturbation theories. The present approach is applied to investigate the electron linewidth from electron-phonon interaction at 0 K and 300 K. It is shown that electron-phonon linewidth in stanene displays an important temperature dependence as a function of electron energy. Two different cases are considered in this report, first for electron state initially at the valence band maximum and second at the conduction band minimum. It is found that the electron-phonon interaction is strongly dependent on the electron wave vector. This orientation dependence can be used as a basis for transport phenomena. The electron scattering rate at room temperature, projected on the six phonons modes, reveals that the contribution is overall dominated by out-of-plane transversal optical modes (*ZO*). Another finding is that stanene's hot carriers thermalize at 250 fs, which is faster than in graphene. This study paves the way to explore hot electrons that are difficult to achieve in experiment.

## 1. Introduction

Recently, graphene has offered novel applications in various fields because of its exceptional properties including high mobility at room temperature, ambipolar effect, Klein tunneling, and anomalous quantum Hall effect [1,2]. This breakthrough spearheaded the creation of new column IV-elements based materials. Silicene, germanene and stanene are honeycomb monolayers that share many similarities with graphene regarding the electron behavior at the Fermi level. In particular, massless Dirac fermions and the linear dispersion-band [3,4]. Unlike graphene which has a planar structure, the large atomic radius of the Si, Ge and Sn atoms makes these 2D materials low buckled. Recent investigations on the growth of Si, Ge and Sn have paved the way for further study of the practical application of low dimensional systems-based devices [5–10].

Graphene, silicene, germanene and stanene are 2D topological insulators whose spin-orbit gap is determined. Compared with graphene, silicene shows a larger spin-orbit coupling strength [16], yielding to a higher gap energy of 1.55 meV at the Dirac point. This spin-orbit band gap can be observed in an experimental accessible low temperature regime [16]. For germanene, the spin-orbit coupling induces a gap energy of 23.9 meV at 277 K [16], while stanene films are the largest gap topological insulators with a gap of 72 meV [17–19]. The larger atomic number of atoms in these materials makes the spin-orbit coupling much stronger, which results in the increasing of the band gap at the Dirac points. On the other hand, appropriate chemical functionalization can widen the stanene gap up to 300 meV under the effect of fluorination, or become a trivial insulator by hydrogenation [20].

In 2015, the stable epitaxial growth of high purity stanene on a $Bi_2Te_3$(1 1 1) substrate was realized from the effusion cells by using MBE method on the Si (1 1 1) wafer [21]. This experiment renders stanene feasible use as topological insulator [22]. Since then, special attention has been devoted to stanene, which has a versatility for (i) enhanced thermoelectric performance near room temperature [23,24], (ii) anomalous quantum effect [25] and (iii) topological superconductivity. Indeed, stanene is a topological insulator that supports the existence of Majorana edge states and zero energy modes of vortex core [26,27]. At the intrinsic room temperature (300 K), the electrons mobility is dominated by the intervalley scattering process of the transversal acoustical modes [28]. Under complete fluorination, stanene becomes a magnetic topological insulator that can accommodate the quantum Hall effect in the absence of a magnetic field. In fluorostanene, a current flow emerges without any energy loss at the edge of the sample [29]. This property makes stanene fluoride a promising material for applications in dissipationless electronics.

Topological superconductivity is a phenomenon dominated by electron-phonon (e-ph) couplings in 2D materials [30]. These interactions also contribute to optical absorption in the indirect gap

* Corresponding author.
*E-mail address:* juniorkanga@ymail.com (N.B.-J. Kanga).

https://doi.org/10.1016/j.commatsci.2018.08.038
Received 18 June 2018; Received in revised form 15 August 2018; Accepted 19 August 2018

semiconductors and give rise to other phenomena such as electrical resistivity, Kohn's effect and polaronic transport [31]. The (e-ph) couplings enable the thermalization of hot carriers and determine the temperature dependence of electronic energy bands [32]. The involvement of the electron-phonon interactions observed in the band structures distortions and the phonon dispersion relations leads to characteristic Raman/neutron spectra [33]. At high temperature, electron thermal transport properties via electron-phonon interaction have shown that thermal conductance in zigzag stanene ribbons (ZSNRs) is superior to that of the zigzag graphene nanoribbons (ZGNRs). This results from lower threshold energies for electron transport modes in ZSNRs [34]. The effects of electron-phonon interactions on the spin-dependent Seebeck effect as well as on the electron transport were also reported for the case of ZGNRs [35,36].

Due to the fundamental and practical importance of the interaction between electrons and the quantized lattice vibrations in 2D materials, we focus our interest to the case of stanene in the absence of spin-orbit coupling. The electron-phonon coupling properties of stanene are investigated by using ab initio techniques and going beyond the limited calculations that use empirical pseudopotentials [37]. It is therefore crucial to resort to Quantum espresso and the Wannier function, which consider additional details to evaluate the imaginary self energy projected on different vibrational modes and its corresponding hot electron scattering rate [38]. This technique provides with a good accuracy, along different crystallographic directions, the electron phonon linewidth with respect to the electron energy.

This work presents a detailed study of the hot electron in stanene by mean of an electron-phonon linewidth. The matrix elements in the conduction band minimum (CBM) and the valence band maximum (VBM) are determined along the entire high symmetry line as a function of the six phonon modes. For the six phonon branches in stanene it is shown that the e-ph imaginary self energy has characteristic dispersions. The electron linewidth and its corresponding scattering rate are carried out with a mapping of this quantity on the high symmetry line of the Brillouin zone (BZ). The results show that the e-ph coupling varies over the entire very dense BZ grid and is dominated mainly by the out-of-plane transversal phonon mode at the conduction band minimum and the valence band maximum. Furthermore, this coupling is very sensitive to the temperature due to the absence of the gap. At K point, the linewidth is almost zero and remains very weak with increasing temperature. This behavior is due to the absence of the electronic states near the Fermi level in stanene.

This paper is organised as follows. In Section 2, we give details on the computational method used. Then, we provide a complete description of the behavior of the stanene linewidth with respect to the electron energy and the temperature. Then, we show the contribution of each phonon modes in the scattering rate as well as the electron self-energy along the high symmetry line. We end with a conclusion.

## 2. Computational method

The calculations reported in this work have been performed for hexagonal stanene with a lattice parameter $a = 4.68$ Å, the tin-tin bond length is $d = 2.8$ Å. Unlike graphene, stanene is buckled with a buckling $\Delta = 0.87$ Å as depicted in Fig. 1. The ground-state electronic structure is computed within Generalized Gradient Approximation (GGA) [39] as implemented in Quantum ESPRESSO code [40]. A cutoff energy for the plane wave basis set of $60Ry$ and norm-conserving pseudo-potentials are used. To simulate the imaginary part of the e-ph self energy ($Im(\sum_{n,\mathbf{k}}^{e-ph})$), the electron-phonon coupling are considered using the EPW program [41]. The ($Im(\sum_{n,\mathbf{k}}^{e-ph})$) is given by [42]:

$$Im\left(\sum_{n,\mathbf{k}}^{e-ph}\right) = \sum_{m,\lambda,\mathbf{q}} |g_{n,m,\mathbf{k}}^{\lambda,\mathbf{q}}|^2 Im\left[\frac{N_{\lambda,\mathbf{q}} + 1 - f_{m,\mathbf{k}}}{\epsilon_{n,k} - \epsilon_{m,\mathbf{k}+\mathbf{q}} - \hbar\omega_{\lambda,\mathbf{q}} - i\eta} + \frac{N_{\lambda,\mathbf{q}} - f_{m,\mathbf{k}}}{\epsilon_{n,k} - \epsilon_{m,\mathbf{k}+\mathbf{q}} + \hbar\omega_{\lambda,\mathbf{q}} - i\eta},\right] \quad (1)$$

where $\hbar\omega_{\lambda,\mathbf{q}}$ is the phonon energy polarized on $\lambda$ direction and $\mathbf{q}$ is the wave vector in the BZ. The $f_{m,\mathbf{k}}$ and $N_{\lambda,\mathbf{q}}$ denote Fermi Bose occupation numbers and $\eta$ is a Lorentzian broadening parameter. The e-ph matrix $g_{m,n,\mathbf{k}}^{\lambda,\mathbf{q}}$ elements are defined by [42]:

$$g_{m,n,\mathbf{k}}^{\lambda,\mathbf{q}} = \langle \psi_{m,\mathbf{k}+\mathbf{q}} | \partial_{\lambda,\mathbf{q}} V | \psi_{n,\mathbf{k}} \rangle, \quad (2)$$

where $m$ and $n$ are the initial and the final electron band indices with wavevectors $\mathbf{k}$ and $\mathbf{k} + \mathbf{q}$, respectively and $\psi_{n,\mathbf{k}}$ is the Kohn-Sham wave function. Over all the phonon modes of the polarization $\lambda$ and the wave vector $\mathbf{q}$, the variation of the Kohn-Sham potential is denoted by $\partial_{\lambda,\mathbf{q}}$.

In order to approximate the energy-conserving $\delta$-function, Gaussian of width 0.005 eV is used. According to [43,46], the Dirac delta-function in the energy conservation is replaced with a Lorentzian with a broadening parameter $\eta$ as expressed in Eq. (1). The relation between the e-ph scattering rate and the imaginary self energy is given by [42]:

$$\tau_{n\mathbf{k}}^{e-ph} = \frac{2(Im(\sum_{n\mathbf{k}}^{e-ph}))}{\hbar}, \quad (3)$$

The electronic and the vibrational states are computed using a dense k-point grid of $32 \times 32 \times 1$ and $16 \times 16 \times 1$ $\mathbf{q}$-points grids. The matrix element are evaluated over a grid of $360 \times 360 \times 1$ $\mathbf{q}$-points to deduce the imaginary part of the self-energy ($Im(\sum_{n\mathbf{k}}^{e-ph})$) within EPW [41].

## 3. Results and discussion

In this section, we focus on the electron linewidth due to the electron-phonon interaction. This key quantity, referred to as $\Delta E$ is related to the scattering rate. In general, $\Delta E$ is given by the uncertainty principle for energy and time $\Delta E \times \Delta t \approx \frac{\hbar}{2}$. Here, the lifetime $\Delta t$ represents how long the electron will remain in the excited state. From this expression, it is obvious that the higher the linewidth, the shorter the lifetime. Therefore, in term of the notations of this work, Eq. (3), that gives the linewidth $Im(\sum_{n\mathbf{k}}^{e-ph})$ in terms of the scattering rate $\tau_{n\mathbf{k}}^{e-ph}$ corresponding to the inverse of the lifetime, can be easily deduce from the uncertainty principal. The analysis of the imaginary part of electron self-energy $\sum_{n\mathbf{k}}^{e-ph}$, expressed in Eq. (1), provides information on the rate of e-ph processes responsible for hot carrier thermalization. According to [42], the evaluation of the electron linewidth requires to consider simultaneously matrix elements between electron and phonon, energy conservation and phase space occupation. Fig. 2 displays the pooling of the electronic band structure of stanene and the imaginary self energy ($Im(\sum_{n\mathbf{k}}^{e-ph})$) on a fine electron wavevector $k$-grid for two different temperatures namely, 0 K and 300 K.

At a temperature of 0 K, the variation of electron linewidth as a function of the electron energy is plotted in Fig. 2a along the $k$-points on the high symmetry line. In this case, the lattice vibration is very weak. Thus, the dominant phenomenon is the phonon emission in combination with the electronic structure of stanene. At $K$-point, a value of 0.005 eV for the $\delta$-function width gives the expected very small value of the linewidth at the VBM and CBM. This can be attributed to the very small contribution in the electronic state near the Fermi level. For upper bands, $Im(\sum_{n\mathbf{k}}^{e-ph})$ has considerable value. The relevant feature of $Im(\sum_{n\mathbf{k}}^{e-ph})$ in stanene appears when the temperature is increased. In order to investigate hot carrier behavior in stanene at room temperature, we choose 300 K rather than other temperature. At 300 K, Fig. 2b shows that the imaginary self energy is very sensitive to the temperature in the conduction bands compared to valence bands. This is due to the fact that, the carrier in the conduction band are free to move which makes them very suggestible to any external perturbation such as