Tunable nonlinear optical response of silicene in terahertz regime

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***Abstract*—The nonlinear optical response of silicene in terahertz (THz) regime is theoretically studied. Since the intrinsic spin-orbit coupling gap of silicene is in the order of 1 THz, the optical response in few THz frequency regime is strongly enhanced by linear and nonlinear conductivity peaks. Furthermore, these conductivity peaks are gate-tunable. The frequency-tripling nonlinear optical current can be significantly larger than the single-frequency current under a moderate electric field strength of 1000 V/cm. This suggests that tunable strong THz frequency-tripling effect can be achieved in silicene.**

I. Introduction and Background

SILICENE is a graphene-like two dimensional structure made up of silicon atoms [1]. Similar to graphene, the low energy electrons residing at the K and K' points of the Brillouin zone are described by the Dirac equation. However, silicene contains richer physical properties than graphene due to the buckled hexagonal lattice structure. The lattice buckling allows a continuously tunable sublattice asymmetry gap to be created via electrical gating. Furthermore, the sp2-sp3 mixed hybridization due to lattice buckling opens up a relatively larger intrinsic SOC gap of $\Delta_{SO} \approx 3.9$ meV [2] in comparsion with graphene ($\Delta_{SO} \approx 1\mu$ eV [3]). Since Δ_{SO} sits around 1 THz, the optical response of silicene is expected to exhibit rich features in few THz regime. In this work, we study the nonlinear optical response of silicene in terahertz frequency regime. We found that the optical response is gate-tunable and is strongly enhanced by the nonlinear optical process.

II. Formalism

The low energy effective tight binding Hamiltonian of silicene is given as [4]

$$\hat{H}_{\tau\sigma}(\boldsymbol{p}) = \begin{pmatrix} -\Delta_{\tau\sigma} & v_F(\tau p_x - ip_y) \\ v_F(\tau p_x + ip_y) & \Delta_{\tau\sigma} \end{pmatrix} \quad (1)$$

where $\Delta_{\tau\sigma} = \tau\sigma\Delta_{SO} - \Delta_z$ and $\Delta_z = eE_z d$. E_z is an out-of-plane electric field and $d \approx 0.46\mathring{A}$ is the out-of-plane buckling distance. The spin and valley are denoted by $\sigma = \pm1$ and $\tau = \pm1$ respectively. The energy dispersion of Eq. (1) is $\varepsilon_{\tau\sigma}(s,\boldsymbol{p}) = s\sqrt{v_F^2 p^2 + \Delta_{\tau\sigma}^2}$. With finite electric gating ($\Delta_z \neq 0$), the spin and valley degeneracies are broken and the bandgap $\Delta_{\tau\sigma}$ becomes electrically tunable. The optical current generated by an in-plane electric field $\boldsymbol{E} = \boldsymbol{E}_0 e^{i\omega t}$ can be calculated by performing a Floquet expansion on the photon-dressed electronic wavefunction: $\Psi_{\tau\sigma}(s,\boldsymbol{p}) = \sum_{n=0}^{\infty}(a_{\tau\sigma}^{(n)}, b_{\tau\sigma}^{(n)})^T$ [5], [6]. The Floquet components, $a_{\tau\sigma}^{(n)}$ and $b_{\tau\sigma}^{(n)}$, can be obtained by solving the Schrodinger equation $i\hbar\partial\Psi_{\tau\sigma}/\partial t = \hat{H}_{\tau\sigma}(\boldsymbol{p}+e\boldsymbol{A})\Psi_{\tau\sigma}$ where $\boldsymbol{E} = -\partial\boldsymbol{A}/\partial t$. Finally, the optical current can be determined from $J(\omega) = \int d\boldsymbol{k}\Psi_{\tau\sigma}^{\dagger}\hat{\boldsymbol{v}}\Psi_{\tau\sigma}\tanh\left(\varepsilon_{\tau\sigma}/2k_BT\right)$ where $\hat{\boldsymbol{v}} = \partial\hat{H}_{\tau\sigma}/\partial p_x$.

III. Results

The optical spectrum of silicene is shown in Fig. 1. The frequency-tripling conductivity $\sigma_{3\omega}$ is significantly stronger than the single-frequency conductivity σ_ω under a moderate electric field strength of 1000 V/cm. Furthermore, the onset frequency of $\sigma_{3\omega}$ is lower than that of σ_ω. This indicates the generation of a purely frequency-tripled optical current in the frequency range covering 0.6 THz to 2 THz.

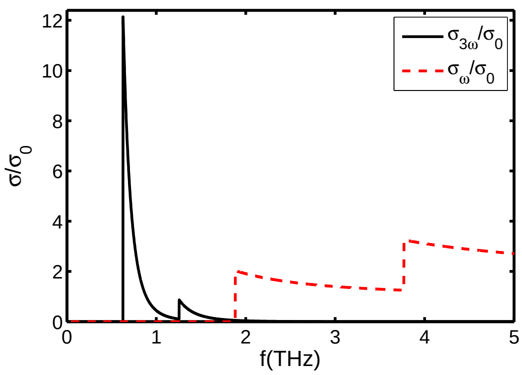

Fig. 1. Single-frequency σ_ω and frequency-tripling $\sigma_{3\omega}$ of silicene at $T = 4$ K, $E = 1000$ V/cm and $\Delta_z = 3\Delta_{SO}$.

IV. Conclusion

The optical response of silicene is strongly enhanced by nonlinear response in THz frequency regime. The gate-tunablity of the optical response can potentially be harnessed to develop silicon-based THz up-converter and detector.

References

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