Optical Hall effect in graphene by strain engineering

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Observation of $V_H$ (along Oy) when $I$ (along Ox) and $B$ (along Oz) are applied

Hall current

$J_y = \sigma_H E_x$

Hall conductivity
Interaction between light and charge carriers

- Incident light
- Transparent material
- Reflected light
- Absorption
- Transmitted light
**Introduction: optical Hall effect**

Interaction between light and charge carriers

- Reflected light
  - Kerr effect (polarization rotated)

- Linearly-polarized incident light

- Optical absorption

- Transmitted light
  - Faraday effect (polarization rotated)

**Optical absorption**:

\[ 1 - T(\omega, B) \approx 2 Z_0 f_s(\omega) \Re \left[ \sigma_{xx}(\omega, B) \right] \]

**Polarization rotation**:

\[ \theta(\omega, B) \approx Z_0 f_s(\omega) \Re \left[ \sigma_{xy}(\omega, B) \right] \]

External magnetic field \( B \) → optical Hall conductivity \( \sigma_{xy}(\omega, B) \)
Introduction: **optical properties of graphene**

**Optical spectra:**
PRL 106, 046401 (2011)

**Magneto-optical effects:**
Nat. Phys. 7, 48-51 (2011)

Faraday rotation
Introduction: **optical properties of graphene**

**Effects of strain:**

EPL 92, 67001 (2010): theoretical


\[ \text{strain} \quad \varepsilon = 0.5\% \]
Motivation: optical Hall effect in strained graphene?

**B-field:**
- time reversal symmetry breaking
- optical Hall effect

**Strain:**
- lattice symmetry breaking
- zero-field optical Hall effect???
Model and methodologies

- Uniaxial strain: magnitude $\varepsilon$ & direction $\theta$
- Light: frequency $\omega$ & polarization $\phi$

**Calculation methods:**

- Density functional theory (DFT) with the SIESTA code
- Semi-empirical tight-binding (TB) method with the Kubo formula:

$$\sigma_{pq}(\omega) = \frac{2e^2}{iS} \sum_{k \in BZ} \sum_{n,m} \frac{f(E_n) - f(E_m)}{E_n(k) - E_m(k)} \frac{\langle n | \hat{v}_p | m \rangle \langle m | \hat{v}_q | n \rangle}{\hbar \omega + E_n(k) - E_m(k) + i \eta}$$

Nguyen et al., 2D Materials 4, 025041 (2017)
Results: optical Hall conductivity in strained graphene

unstrained graphene:
- zero optical Hall conductivity $\sigma_{xy} = 0$

strained graphene:
- VHS peaks of $\sigma_{xx}$ are separated
- finite optical Hall conductivity
  $\sigma_{xy} > 0$ for low $\omega$
  $\sigma_{xy} < 0$ for high $\omega$
Results: **optical Hall conductivity in strained graphene**

- 2 distinguishable K-points
- 3 distinguishable M-points

conduction bands
**Results:** optical Hall conductivity in strained graphene

Kubo formula for optical conductivities

\[ \sigma_{pq}(\omega) = \frac{2 e^2 \hbar}{i S} \sum_{k \in BZ} \sum_{n,m} \frac{\langle n | \hat{v}_p | m \rangle \langle m | \hat{v}_q | n \rangle}{\hbar \omega + E_n(k) - E_m(k) + i \eta} \]

with \[ C_{pq}(k) = \langle n | \hat{v}_p | m \rangle \langle m | \hat{v}_q | n \rangle \]
Results: optical Hall conductivity in strained graphene

Kubo formula for optical conductivities

\[ \sigma_{pq}(\omega) = \frac{2e^2 \hbar}{iS} \sum_{k \in BZ} \sum_{n,m} \frac{\langle n|\hat{\psi}_p|m\rangle\langle m|\hat{\psi}_q|n\rangle}{\hbar \omega + E_n(k) - E_m(k) + i\eta} \]

with

\[ C_{pq}(k) = \langle n|\hat{\psi}_p|m\rangle\langle m|\hat{\psi}_q|n\rangle \]

conduction bands

coefficient \( C_{xy}(k) \rightarrow \sigma_{xy} = \sigma_{xy}^+ - \sigma_{xy}^- \)
Results: **possible large values of** $\sigma_{xy}$

1. **large values** $\sigma_{xy} \sim 1÷2 \sigma_0$ for small strain of ~ a few %
2. $\sigma_{xy} \propto$ number of layers $N_L$
3. sign of $\sigma_{xy}$ can be reversed by tuning not only $\omega$ but also strain type (positive $\varepsilon$ or negative $\varepsilon$)
Results: direction dependence of $\sigma_{xy}$

- $\sigma_{xy}$ depends only on $\omega$ and $\varepsilon$ but also light polarization $\phi$ and strain direction $\theta$
- $\sigma_{xy}$ generally exhibits three peaks but only two if $\phi$ or $\theta \equiv$ armchair/zigzag direction
Results: **direction dependence of $\sigma_{xy}$**

\[ \hbar \omega = 1.5 \text{ eV} \]

\[ \hbar \omega = 3.2 \text{ eV} \]

\[ \sigma_{xy} \propto \sin(2(\phi - \theta)), \quad \text{i.e., small if } \phi - \theta \approx n\pi/2 \]

and have peaks when \( \phi - \theta \approx n\pi/2 + \pi/4 \)
Results: optical Hall effect in other materials

strain engineering: a common technique to generate optical Hall effect!!!
- strain engineering: general/alternative approach to achieve optical Hall effect
- both value and sign of $\sigma_{xy}$ are tunable by strain ($\varepsilon, \theta$) and incident light ($\omega, \phi$)

=> possible opto-electro-mechanical applications:
  e.g., AC Hall systems, optical modulators, sensors, rotators, polarizers?
Conclusion

Faraday rotation

- Low energy lights

- High energy lights
- strain engineering: general/alternative approach to achieve optical Hall effect
- both value and sign of $\sigma_{xy}$ are tunable by strain ($\varepsilon, \theta$) and incident light ($\omega, \phi$)

$\Rightarrow$ possible opto-electro-mechanical applications:

  e.g., AC Hall systems, optical modulators, sensors, rotators, polarizers?

\[ \sigma_{xy} \propto \sin(2(\phi-\theta)) \]
THANK YOU FOR YOUR ATTENTION