Evidence for Dominant Phonon-Electron Scattering in Weyl Semimetal WP2

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https://journals.aps.org/prx/abstract/10.1103/PhysRevX.11.011017 [1]

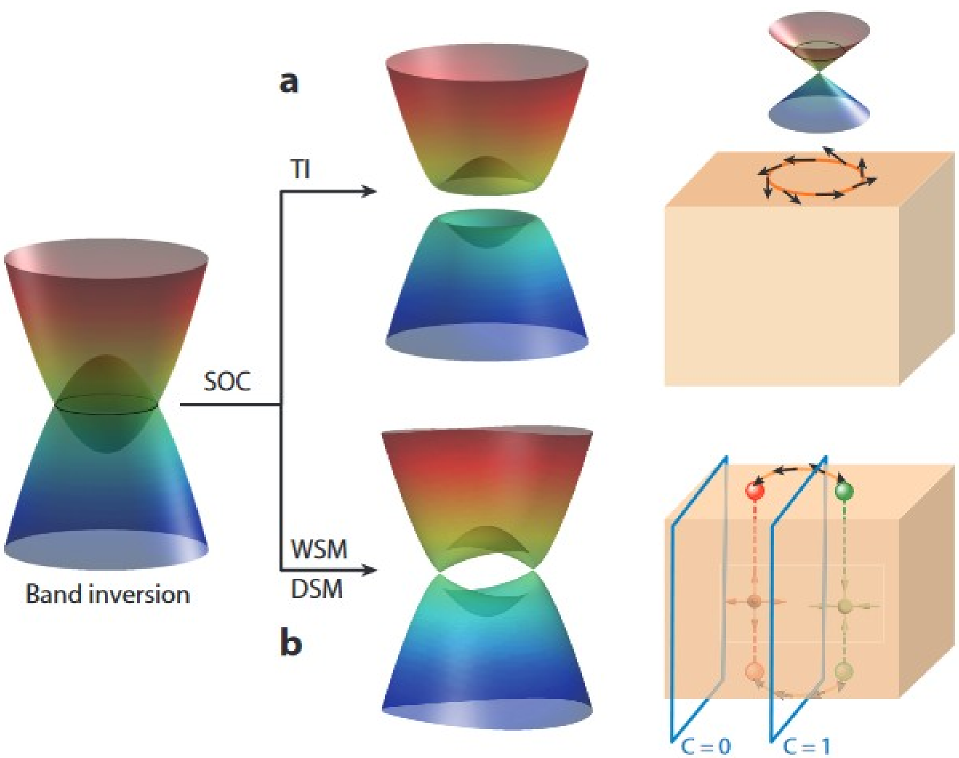
Presentation by: Daniel Hagspihl

18.05.2021

Contents

Topological Materials

- Band structure between Insulator and Conductor
- SOC leads to Band Inversion
- Bands touch: Cones
- TRS or lattice symmetry broken → Weyl Cones
- Else: Dirac Cone (degenerate)



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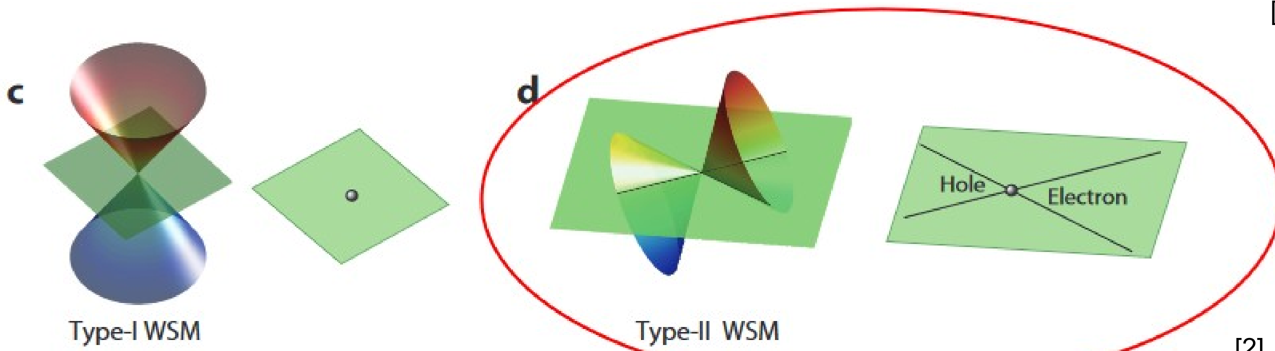
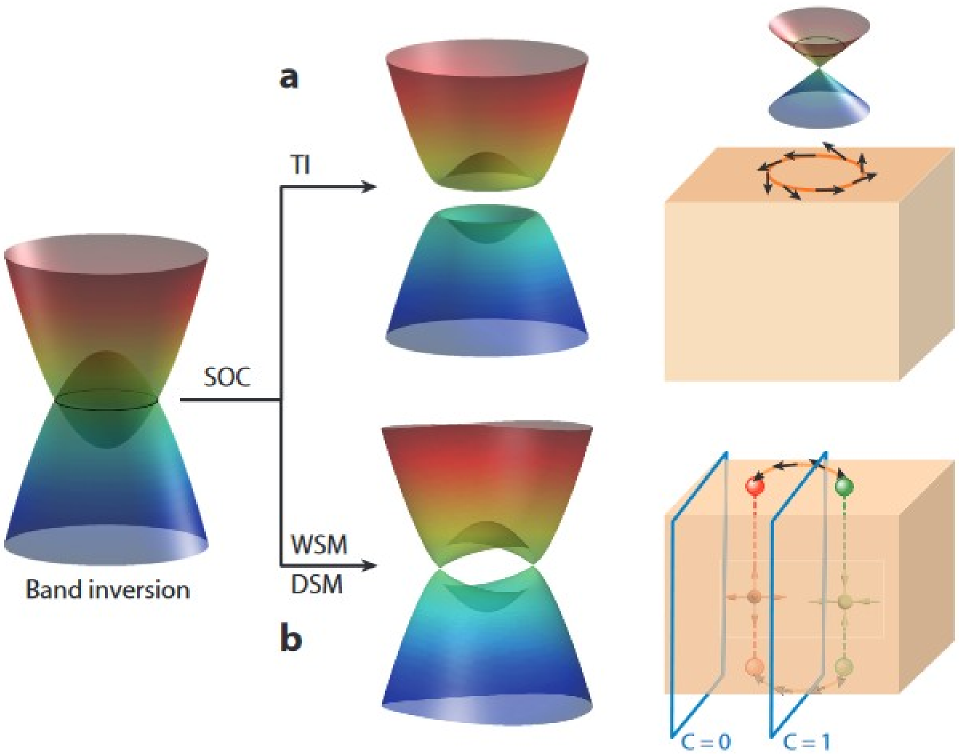


[2]

[2] Binghai Yan, Claudia Felser, *Annu. Rev. Condens. Matter Phys*, **8**, 337-354 (2017)

Weyl Semimetals

- WSM: Topological states on the surface (Fermi arcs in contrast to closed Fermi surface, spin & momentum are locked)
- Chiral magnetic effects inside the material (Weyl cones)
- Extremely high conductivity and magnetoresistance



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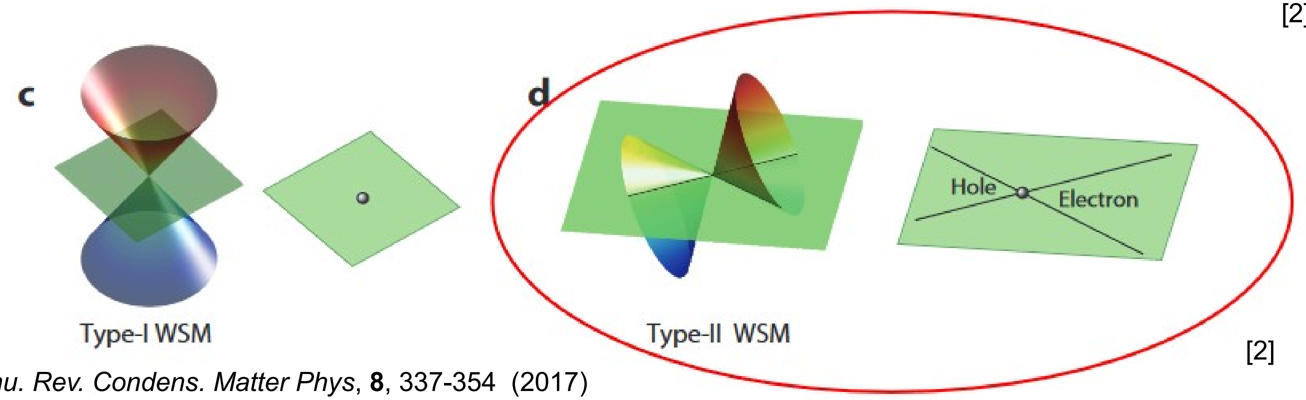


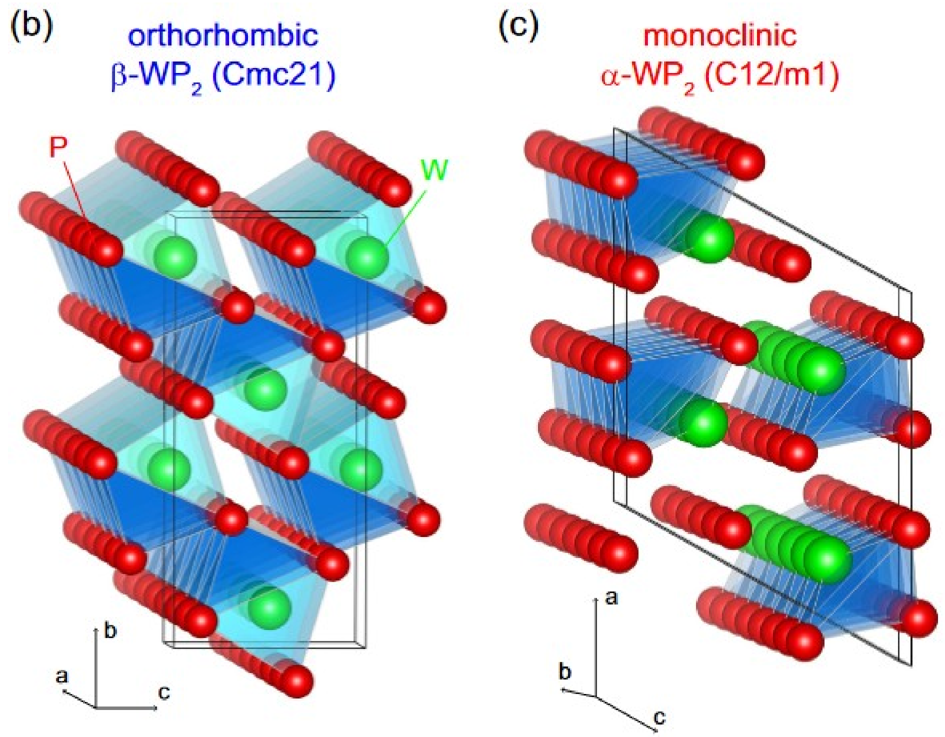
[2]

[2] Binghai Yan, Claudia Felser, *Annu. Rev. Condens. Matter Phys*, **8**, 337-354 (2017)

ß-WP_2

No lattice symmetry

→ WSM

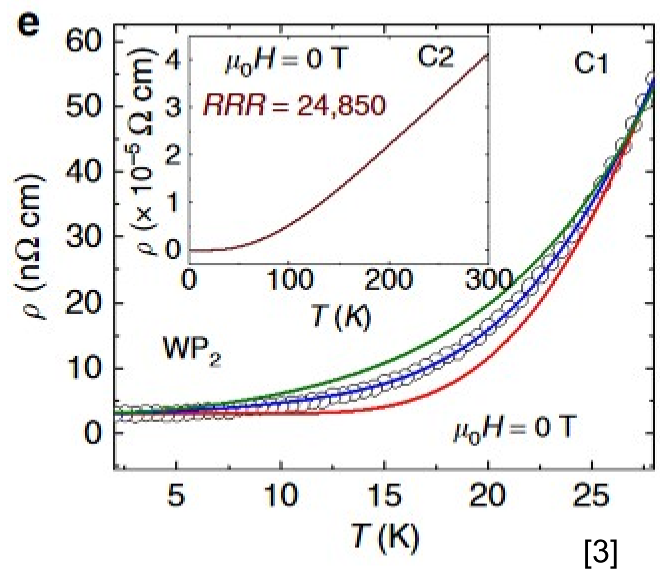


[7]

[7] Dirk Wulferding et al, Phys. Rev. B, **102**, 075116 (2020)

Motivation

- RRR=ρ(300 K)/ρ(2 K) (residual resistivity ratio)
- RRR(WP_2) ≈ 25.000
- RRR(Copperwire) ≈ 40 – 50 [4]
- Green line: impurities, e-e, e-ph:
  $\rho(T)=\rho_0+a\cdot T^2+b\cdot T^5$
- Red line: Phonon drag (ph-e) (e get "dragged along"): normally small, but with suppressed ph-ph decay, ph-e becomes more significant
- $\rho(T)=\rho_0+ c\cdot \exp(-T_0/T)$
- Blue line: combined terms



[3]

[3] Nitesh Kumar et al. *NATURE* (2017)

Motivation

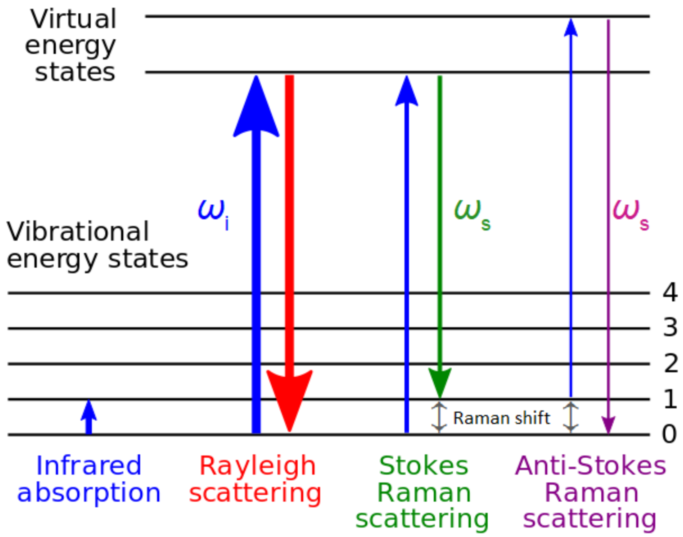
Scattering mechanisms central to the high conductivity largely unexplored.

Idea: momentum lost to phonons (in e-ph) can be regained if these phonons scatter back into electrons (e-ph) signifficantly more then into other phonons (ph-ph)

→ higher conductivity

Raman spectroscopy - Theory

- Incident photon with ω_i excites the energy state
- Most of these states relax back into original state (Rayleigh)
- Some relax into another vibrational state (Stokes/ Anti-Stokes) emitting ω_s
- Raman shift = $|\omega_i - \omega_s|$ is the Energy of the created/ annihilated phonon
- Not only sensitive to ω, but also to k.
- Only optical Phonons can be observed

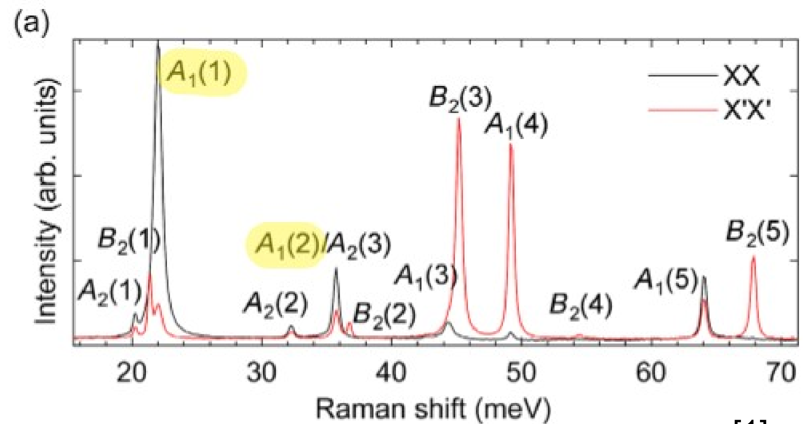


[5]

[5] https://en.wikipedia.org/wiki/Raman_spectroscopy (12.5.2021)

Raman spectroscopy

Raman spectroscopy to see the different phonon modes



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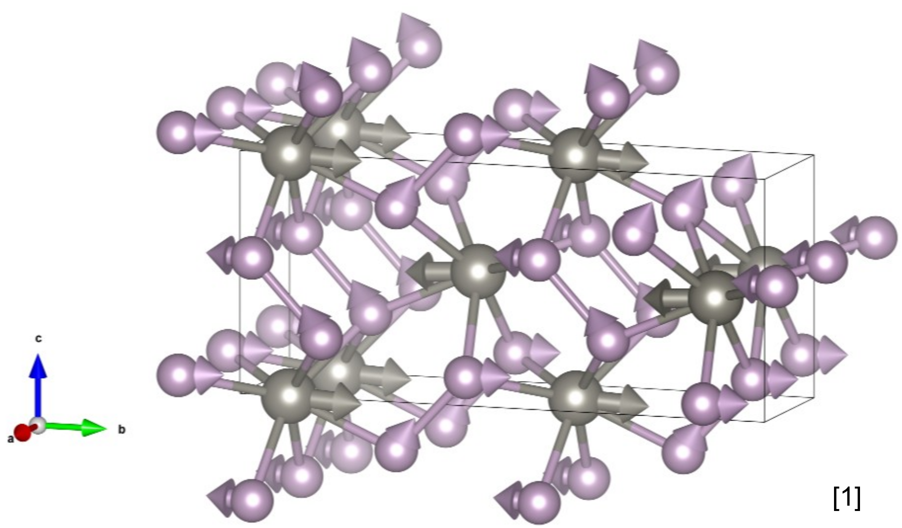
Example: displacements of $A_1(1)$ mode



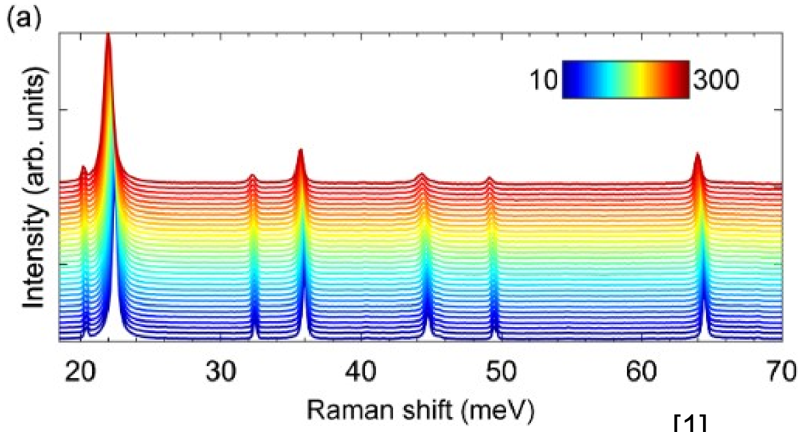
[1]

[1] Gavin B. Osterhoudt et al., *Phys. Rev. X,* ***11*** *011017* (2021)

Raman spectroscopy

Typically, Phonon Energy decreases with increasing Temperature

(lattice expansion → Phonons have larger wavelength)



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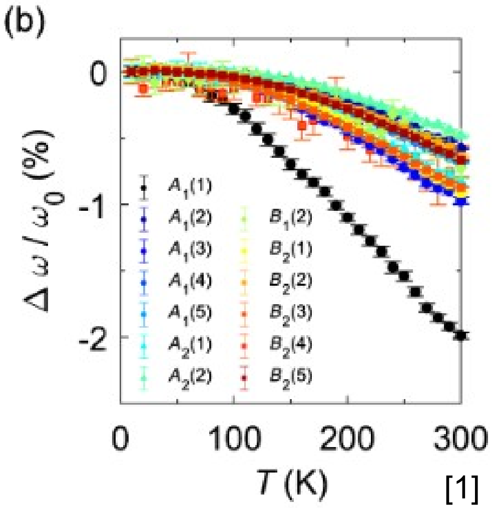


[1]

Percentage change of each modes energy.

Most modes change by 1% while $A_1(1)$ changes by 2%.

[1] Gavin B. Osterhoudt et al., *Phys. Rev. X,* ***11*** *011017* (2021)

Phonon Linewidth Measurements

Linewidth is dependant on the Lifetime of the Phonon (uncertainty Principle):

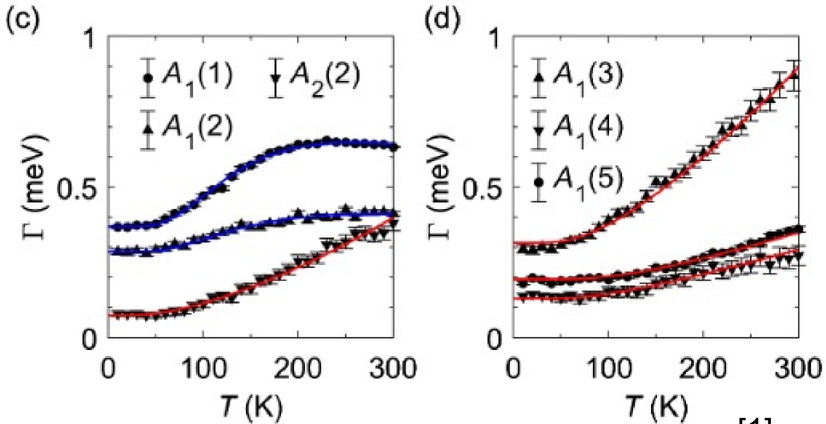
- Long Lifetime ↔ small Linewidth
- Short Lifetime ↔ big Linewidth

Temperature dependence of ph-ph decay is governed by Bose-Einstein distribution

Higher $T \rightarrow$ higher density of states $\rightarrow$ more scattering

$\rightarrow$ linewidth increases monotonically with T

Doesn't fit the observation for $A_1(1)$ and $A_1(2)$



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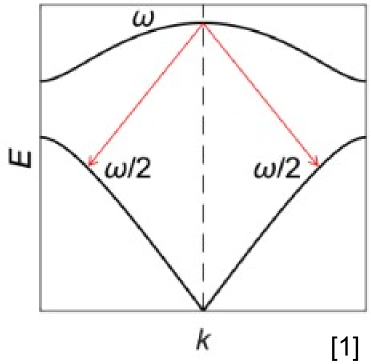


[1]

[1] Gavin B. Osterhoudt et al., *Phys. Rev. X,* ***11*** *011017* (2021)

Phonon Linewidth Measurements

Model for ph-e decay:

Decay rate dependent on difference in occupation of states n_I - n_T

in graphene:

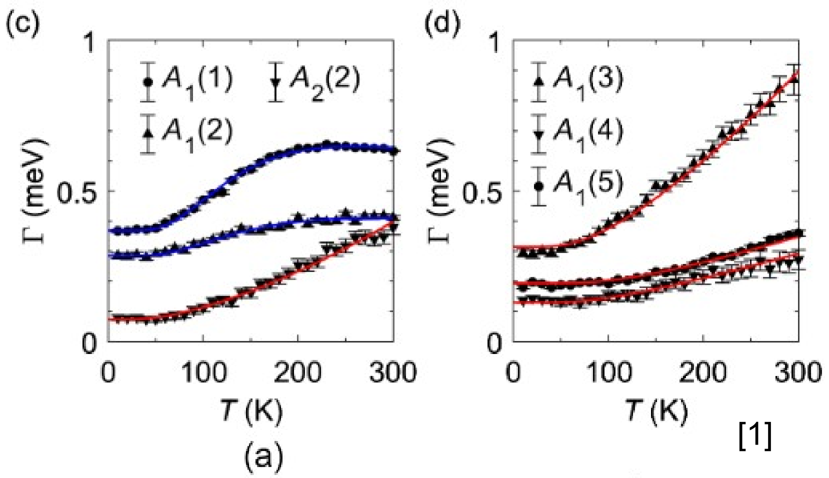
Initial State < E_F

Target occupation higher with bigger T

→ difference in occupation smaller

→ linewidth decreases monotonically with T

Doesn't fit the observation for $A_1(1)$ and $A_1(2)$



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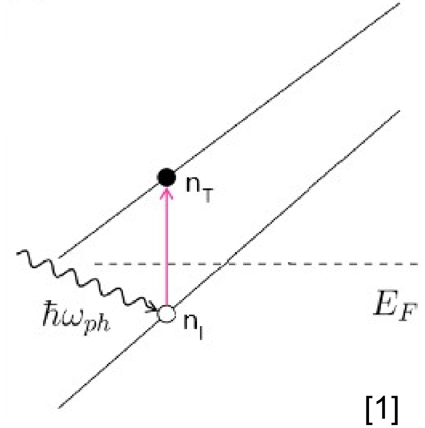


[1]

[1] Gavin B. Osterhoudt et al., *Phys. Rev. X*, ***11*** *011017* (2021)

Phonon Linewidth Measurements

Model for ph-e decay:

Decay rate dependent on difference in occupation of states

New model:

Initial State > E_F

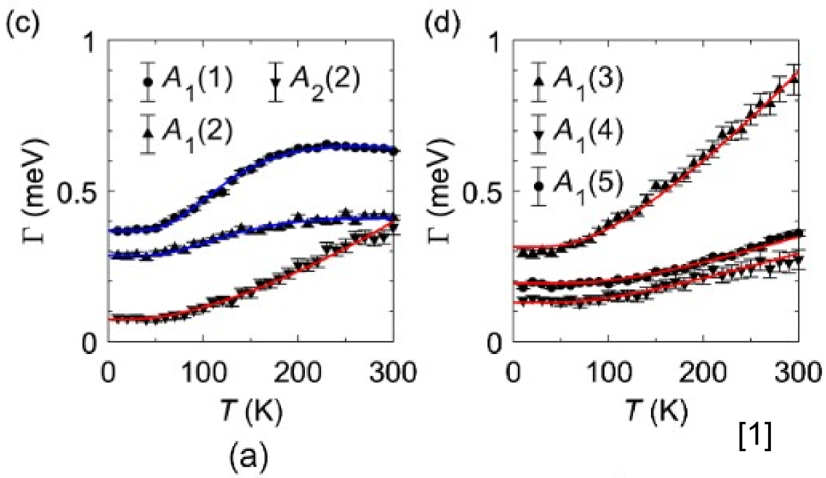
WP2: $\Gamma(T) \propto n_I - n_T$

Since the electron states are ω_a above E_F they are not thermally populated at low T

→ increase at low T, decrease at high T

Matches with behavior of $A_1(1)$ and $A_1(2)$

There are Interband and intraband transitions



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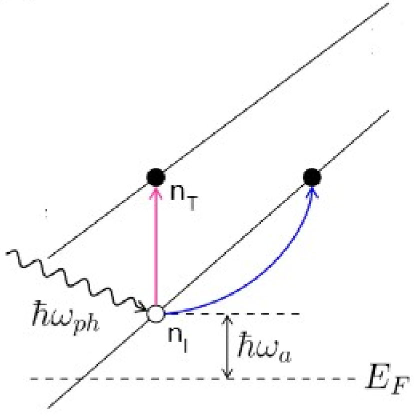
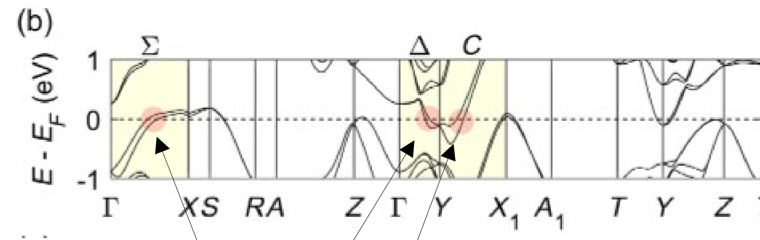


[1]

[1] Gavin B. Osterhoudt et al., *Phys. Rev. X*, ***11*** *011017* (2021)

Energy conservation

The calculated electronic band structure.
∪-shaped Bands: electron-like Bands
∩-shaped Bands: hole-like Bands



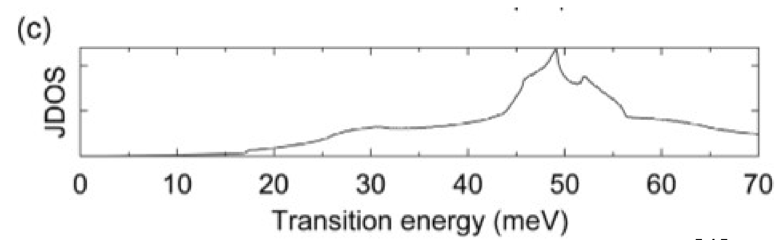
[1]

bands are split
→ gaps are in scale of the optical phonons (70meV)
→ allows $q\approx0$ transitions

Intraband transitionsalways alowed in terms of E
Joint density of states (JDOS) for vertical transitions at low Temperature

- Max between 40-60 meV
- but: A_1(1) and A_1(2) at 22.4 meV & 35.8 meV
- A_1 modes in 40-60 meV have ph-ph decay

→ Conservation of Energy allows the observed transition, but availability of states is not the biggest



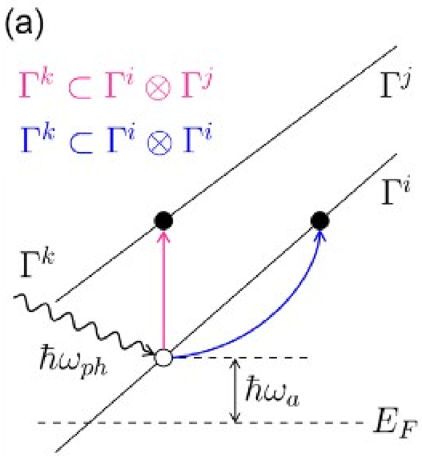
[1]

[1] Gavin B. Osterhoudt et al., *Phys. Rev. X,* ***11*** *011017* (2021)

Selection Rules

Normaly this has do be considered, here the Result is that all transitions are possible.

Interband and intraband likely contribute to the linewidth of $A_1(1)$ and $A_1(2)$.



[1]

[1] Gavin B. Osterhoudt et al., *Phys. Rev. X*, ***11*** *011017* (2021)

Momentum conservation

Interband

transition with q=0 exist for whole range of optical phonon energy. (q≈0 looks similar)

→ momentum conservation trivially fulfilled.

Intraband:

Calculated the max. momentum the Photons can transfer: $q \leq 4\pi n_i(\lambda)/\lambda = 9.68\times10^7\ m^{-1}$

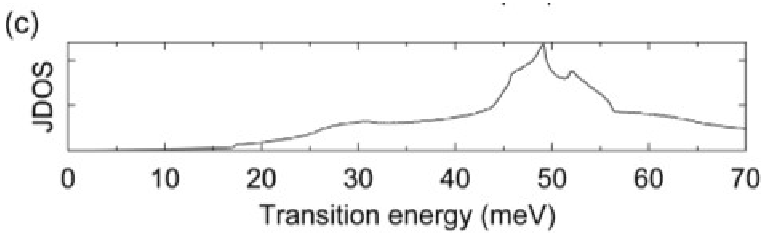
Needed for transfer: $q = \Delta E / (\hbar\, v_F)$

$A_1(1)$ $q \approx 8.57\times10^7\ m^{-1}$ Enough

$A_1(2)$ $q \approx 1.37\times10^8\ m^{-1}$ Not enough (almost, so some are possible)

Higher A_1 modes: $q \approx 1.71\times10^8\ m^{-1}$ Not enough

Might explain why the linewidth of $A_1(1)$ is stronger influenced by the ph-e decay path then $A_1(2)$



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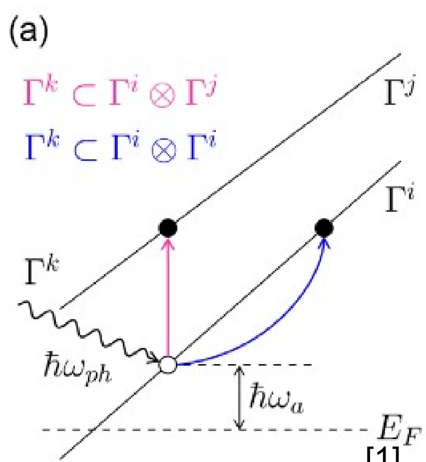


[1]

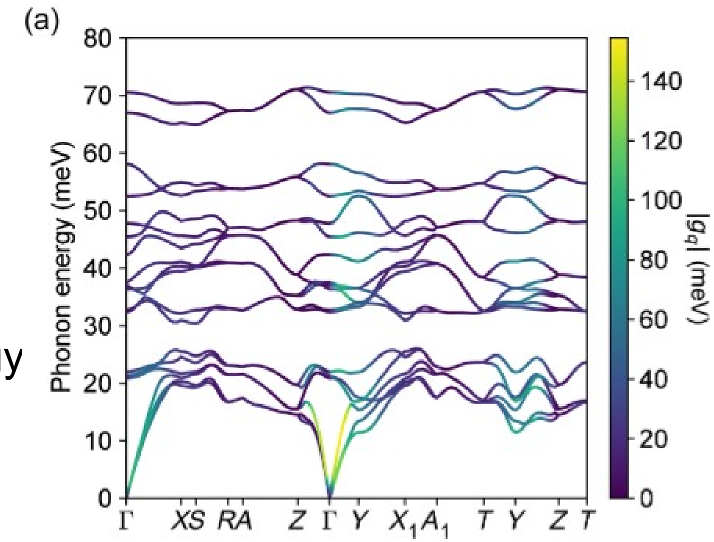
[1] Gavin B. Osterhoudt et al., *Phys. Rev. X,* ***11*** *011017* (2021)

Phonon Electron Coupling

Decay paths available from the Selection Rules for A_2, B_1, B_2, But no anomalous linewidth.

g: electron-phonon-coupling constant (explain color)

g is high near Γ (at finite q near zero) and at low Energy



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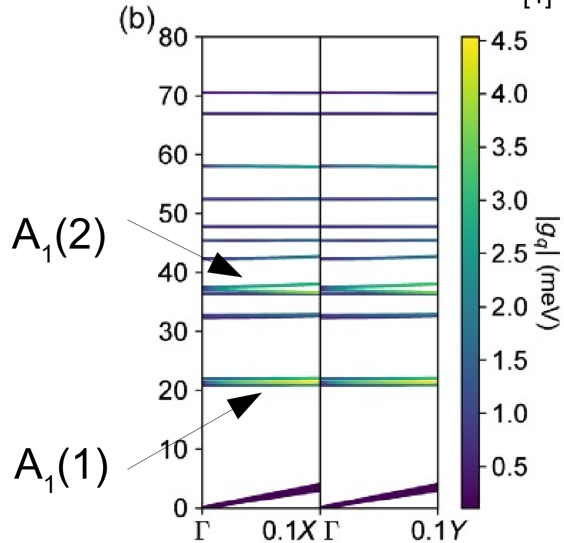
For q=0: phonon electron coupling very weak

For finite q, it rises drastically for $A_1(1)$ and $A_1(2)$ put arrows



[1]

[1] Gavin B. Osterhoudt et al., *Phys. Rev. X*,***11*** *011017* (2021)

Discussion

Why does ph-e dominate over ph-ph?

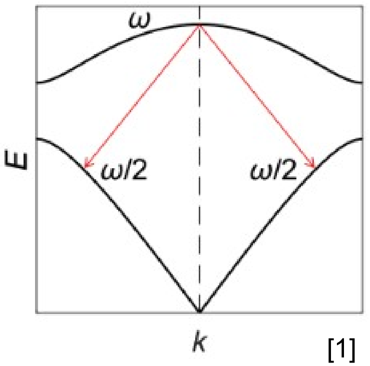
Low E optical ph decays into 2 acoustical ph

lowest Energy optical Phonons are close to the Energy of the acoustic phonons

→ can only decay into really low E acoustic phonons

Density of states increases with k

Low amount of decay paths available



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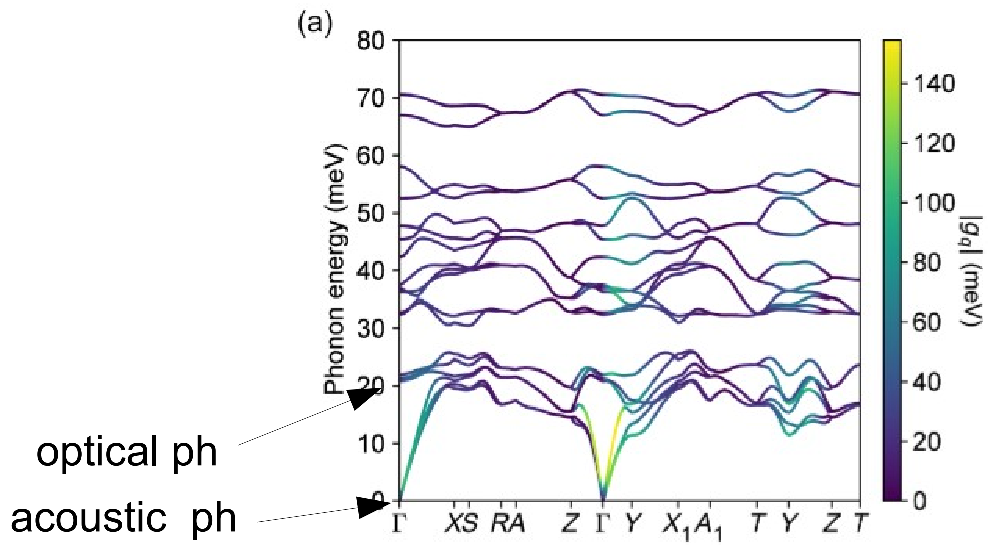


[1]

[1] Gavin B. Osterhoudt et al., *Phys. Rev. X*, ***11*** *011017* (2021)

Discussion

For mobility, acoustic phonons are important, not optical phonons

They calculate the lifetime of of accousstic ph that scatter into e ($\tau_{ph\text{-}e}$) and ph that scatter into ph ($\tau_{ph\text{-}ph}$):

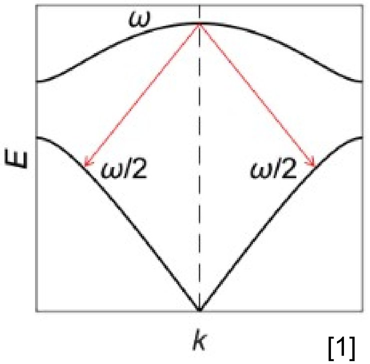
$\tau_{ph\text{-}e}/\tau_{ph\text{-}ph} \approx 0.1$

Same bunching Argument as above

→ strongly suggests dominance of ph-e scattering for acoustic ph as well

Weyl-nodes are hundreds of meV under E_F, so the topological nature of the semimetal might not play a role.

But SOC (which is also the cause for the Weyl-nodes) is important, as it splits the Band.



[1]

[1] Gavin B. Osterhoudt et al., *Phys. Rev. X,* ***11*** *011017* (2021)

Conclusion

Momentum “lost” to phonons by e-ph scattering may be returned to electrons by ph-e scattering, which improves conductivity

→ Consistent with phonon drag effect

It is not known if acoustic Phonons behave the same, as only optical phonons could be observed with the Raman-spectroscopy

Further studies on acoustic phonons needed.

They did not explain a physical background for the positive ω_A

But: α-WP_2 has similar properties (conductivity) but has no SOC and no splitting

Sources:

[1] Gavin B. Osterhoudt et al, Evidence for Dominant Phonon-Electron Scattering in Weyl Semimetal WP2, *Phys. Rev. X,* ***11*** *011017* (2021) https://journals.aps.org/prx/abstract/10.1103/PhysRevX.11.011017

[2] Binghai Yan, Claudia Felser, Topological Materials: Weyl Semimetals, *Annu. Rev. Condens. Matter Phys*, **8**, 337-354 (2017)

[3] Nitesh Kumar et al, Extremely high magnetoresistance andconductivity in the type-II Weyl semimetals WP_2 and MoP_2. *NATURE* (2017)

[4] https://en.wikipedia.org/wiki/Residual-resistance_ratio (12.5.2021)

[5] https://en.wikipedia.org/wiki/Raman_spectroscopy (21.5.2021)

[6] https://www.researchgate.net/figure/Schematics-of-the-topological-insulator-and-Weyl-semimetal-a-A-TI-exhibits-an-energy_fig2_281312307 (23.5.2021)

[7] Dirk Wulferding et al, Effect of topology on quasiparticle interactions in the Weyl semimetal WP2, Phys. Rev. B, **102**, 075116 (2020)

[9] R. Schönemann et al, PHYSICAL REVIEW B, **96**, 121108(R) (2017)

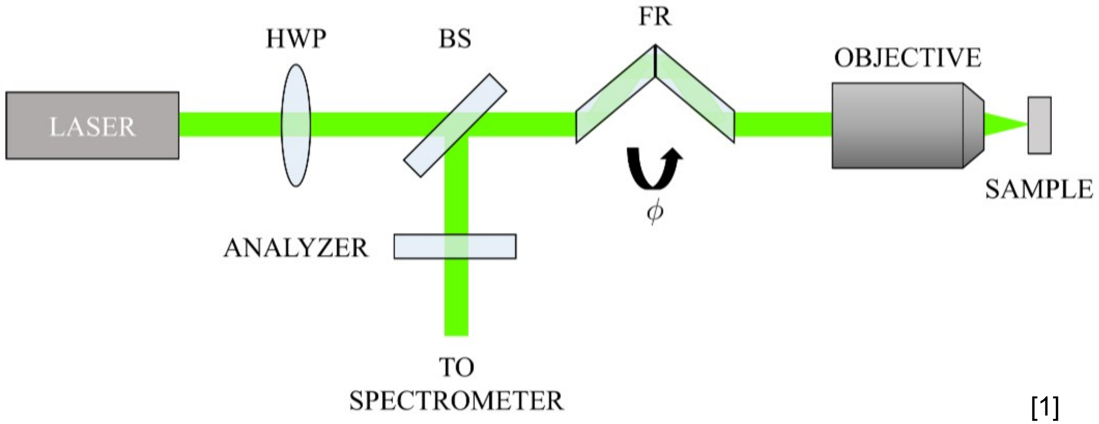
Thank you for listening!

Extra Slides – Raman Scattering

HWP – Half-wave plate

BS – Beam Splitter

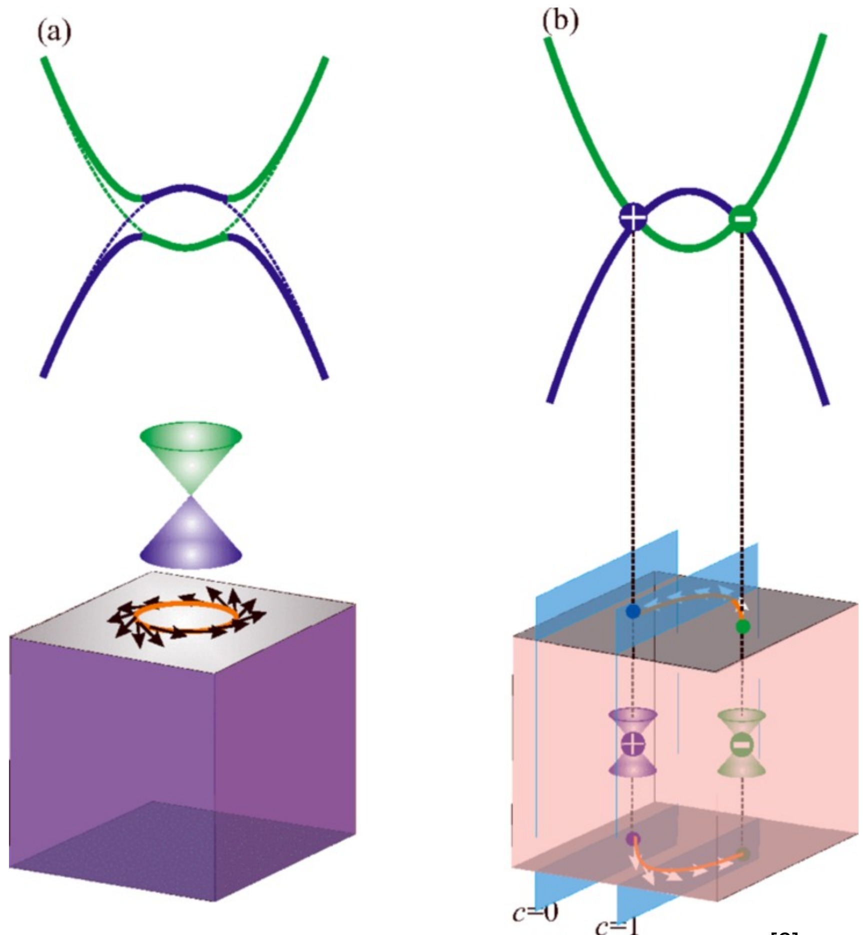
FR – double Fresnel rhomb



[1]

[1] Gavin B. Osterhoudt et al., *Phys. Rev. X,* ***11*** *011017* Supplemental (2021)

Extra Slides – WSM



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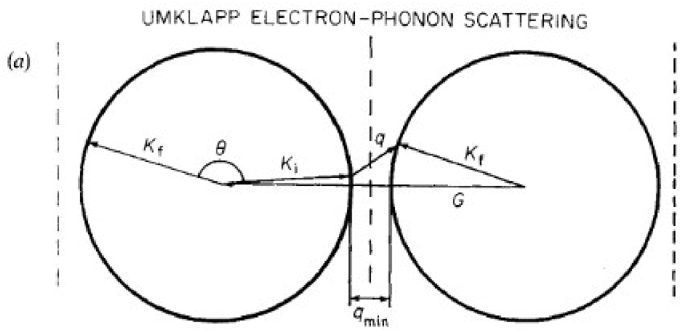
[6] https://www.researchgate.net/figure/Schematics-of-the-topological-insulator-and-Weyl-semimetal-a-A-TI-exhibits-an-energy_fig2_281312307 (23.5.2021)

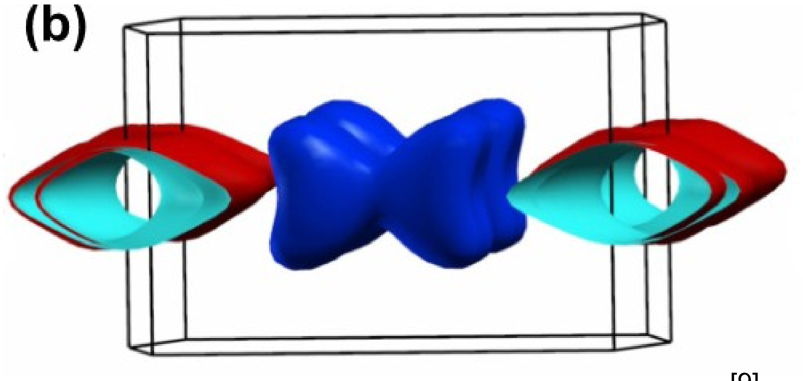
Extra Slides – Umklapp ph-e Scattering



[8]

[8] Nathan Wiser, *CONTEMP. PHYS.*, VOL. 25, NO. 3, 21 1 -249 (1984)

Extra Slides – Fermi Surface of WP_2



[9]

[9] R. Schönemann et al, PHYSICAL REVIEW B, **96**, 121108(R) (2017)