Optical conductivity of high-entropy alloys based on BaMnSb2

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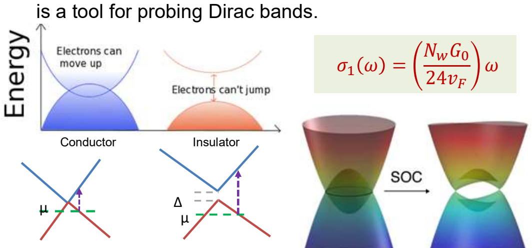
Abstract

The newly discovered Dirac (relativistic) semimetal BaMnSb2 is a potential candidate for energy applications, such as energy harvesting, terahertz detection, high speed electronics and quantum computing. The band gap and other electronic properties can be tuned through various substitutions at the Ba-site. Here, we present low temperature infrared measurements of undoped BaMnSb2 single crystals and those alloyed at the Ba-site with Ca, Eu and Yb, at various individual concentrations. By measuring reflectance spectrum spanning three orders of magnitude in energy, and at cryogenic temperatures (-320F), we explore the electronic properties of this compound.

Background

- In a typical metal or semimetal, energy bands are parabolic and electron spin states are degenerate (indistinguishable).
- In Dirac semimetals, relativistic (Dirac) corrections give rise to linear bands. Additionally, spin orbit coupling (SOC) can produce gapping between bands.
- Absorption between Dirac energy bands are characterized by linear frequency dependence.
- Therefore, optical conductivity (absorption) is a tool for probing Dirac bands.



$$\sigma_1(\omega) = \left(\frac{N_W G_0}{24 v_F}\right)\omega$$

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Experimental Setup

- Single crystals of doped $(Ba_{0.35}Ca_{0.15}Eu_{0.16}Yb_{0.34})MnSb_2$ and undoped $BaMnSb_2$ and were grown by Antu Laha in Zhiqiang Mao's lab at Penn State.
- The samples were small (~2mm diameter) and doped sample was polished on largest flat surface.
- Reflectance was measured in the range 100 cm-1 to 25,000 cm-1 (0.012eV – 3eV), using a VERTEX 70 Bruker FTIR
- Temperatures measured using Janis Optical Flow Cryostat from 300 – 77K.
- Absolute values of reflectance were obtained by measuring coating sample with Au.

Optical conductivity

- Reflectance data we get is a measure of intensity of light
- Phase and intensity are related by Kramers- Kroning relations
- Complex Dielectric Function (N) describes the entire response dynamics of a material to external radiation

$$R = \left|\frac{(1-N)^2}{(1+N)^2}\right| = \frac{(1-n)^2+k^2}{(1+n)^2+k^2} \xrightarrow[\text{Phase}]{\text{Kramers-Kronig}} \theta(\omega) = -\frac{\omega}{\pi} P\int_0^\infty d\omega' \frac{\ln R(\omega')}{\omega'^2-\omega^2} \xrightarrow{\text{Complex Dielectric Function}} N = \sqrt{\tilde{\varepsilon}_r} = n + jk$$

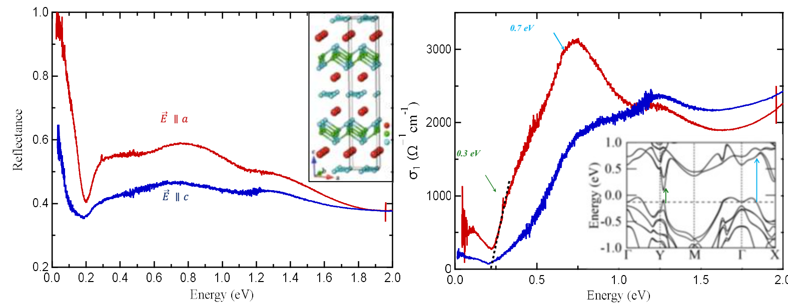
$$\tilde{\varepsilon}_r = \varepsilon_1 + j\cdot\varepsilon_2 = \tilde{\varepsilon}_r = \varepsilon_1 - j\cdot\frac{\tilde{\sigma}(\omega)}{\varepsilon_0\omega}$$

$$\sigma_1 = \frac{\sigma_{DC}}{1+\omega^2\tau^2}$$

- Epsilon 1 (real part) is the polarization of a material under applied light.
- Epsilon 2 describes the loss (scattering)
- Epsilon 2 is written as sigma optical conductivity which is also a complex function.
- Sigma 1 is related to absorption. Most commonly plotted & investigated

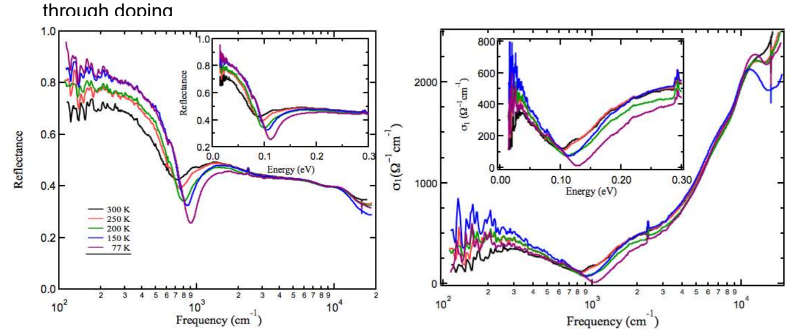
Reflectance Data (undoped sample)

- Strong in-plane anisotropy, similar to previous results: PRB 105, L241110 (2022)
- We observed a sharp conductivity edge, with $\sigma(\omega) \propto \omega$, consistent with Dirac (linear) band dispersion at the Y point.
- Identified interband transitions in good agreement with band structure calculations

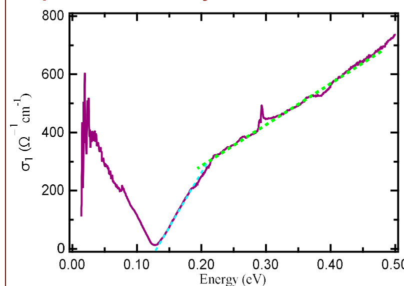


Reflectance Data (doped sample)

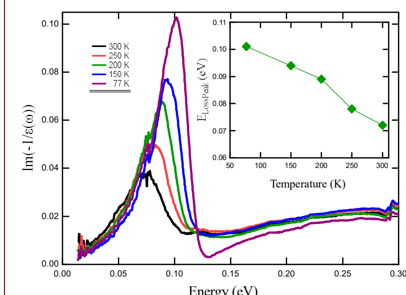
- Sharp plasma edge like in the undoped BaMnSb2
- We still observe a sharp conductivity edge, with $\sigma(\omega)\propto\omega$, but shifted significantly to lower energy: ~ 0.2 eV vs ~ 0.3 eV
- Mid/Near Infrared transitions broaden significantly, consistent with induced disorder through doping



Optical conductivity and Loss Function Data (doped sample)

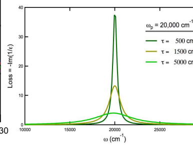


- Clear linear behavior
- Consistent with transitions across Dirac bands
- Dirac bands are preserved
- Peak/dip supposed to stay the same but ours shift to higher frequency

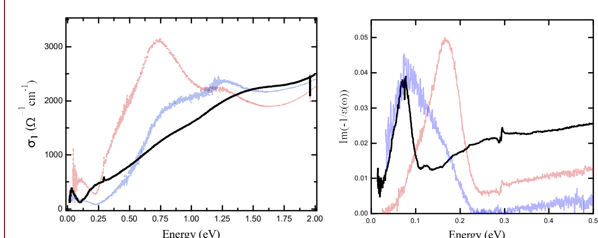


- Loss function gives us a peak at the plasma frequency

$$Loss = -\mathrm{Im}\left(\frac{1}{\tilde{\varepsilon}_r}\right)$$



- In mid IR we see broadening of peaks with is consistent with induced disorder through doping
- Due to unknown axis which sample was polished, we cannot be certain



Conclusions

Using broadband optical spectroscopy, we found that:

- Doping still preserves the linear optical conductivity consistent with Dirac Band dispersion.
- There is still a strong, sharp peak in the loss function which means good conducting behavior.
- Unlike in the undoped case, there is a strong band structure renormalization with temperature.

References

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