ELECTRON-PHONON COUPLING CALCULATIONS OF WEYL SEMIMETAL TAAS

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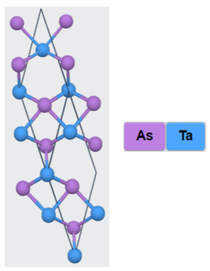
Abstract

Thermoelectric materials are widely used in electronic devices. Due to their high electronic mobility, Weyl semimetals appear to be of great interest for industrial applications because they exhibit a strong positive magneto-conductance. In these materials, electrons can behave as massless chiral fermions (called Weyl fermions) and undergo anomalous transport due to topological features such as band inversion and Weyl points. In order to study these Weyl semimetals, characterize their thermoelectric transport properties and quantify the anomalous transport, we determine their equilibrium geometry and ground state electronic structure and then compute the electron-phonon coupling and phonon limited mobilities. We employ the *Abinit* software suite, implementing DFT, DFPT and transport and apply it in this poster to TaAs, the first experimentally proved Weyl semimetal.

Structure and computational method

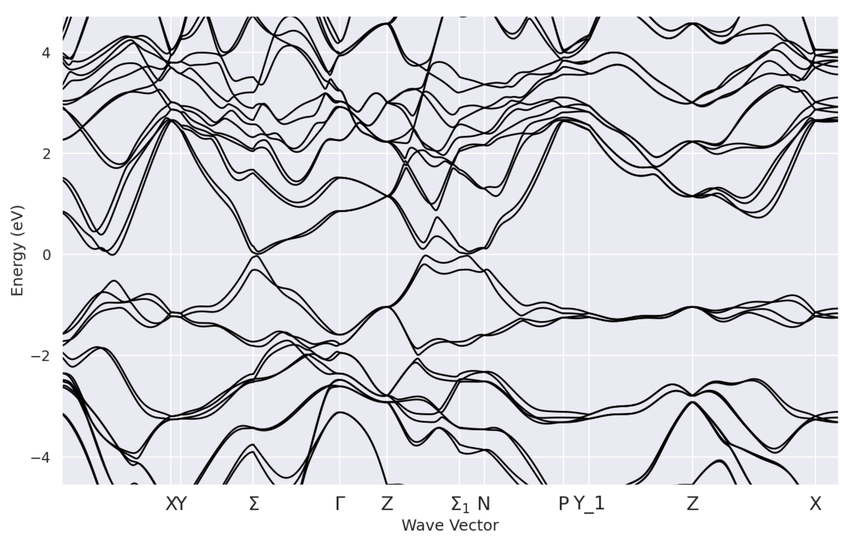


a	b	c	Source
3.274	3.274	11.102	This work
3.467	3.467	11.755	Theory
3.437	3.437	11.656	Exp.

Table 1: Calculated lattice constants (in Å) compared to the literature, theoretical data and experimental data from [1].

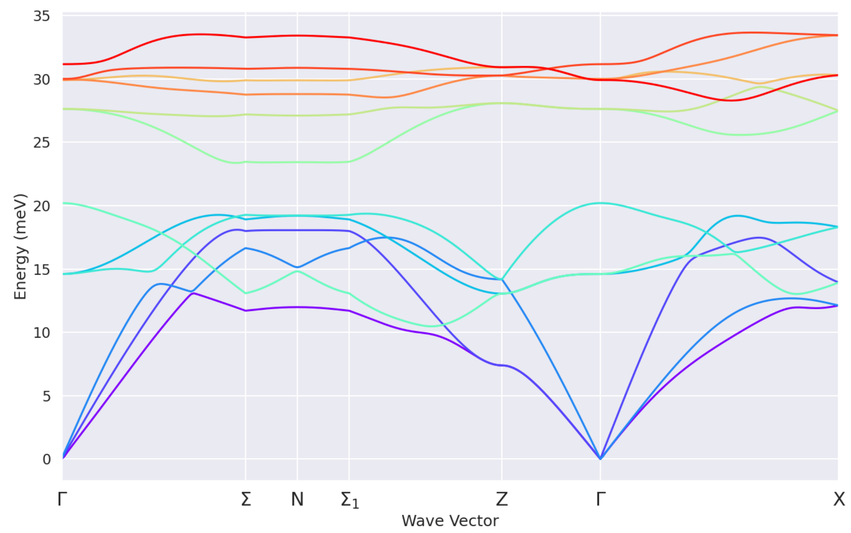
Weyl semimetal TaAs crystallizes in a 4 atom primitive cell. This material has a tetragonal structure (I41md (109) space group) and is non-magnetic. The calculations presented in this poster are performed using an energy cutoff of 35 Ha, GGA and spin-orbit coupling pseudopotentials and a 8x8x8 k-point grid.

Electronic band structure



The bands cross in the vicinity of the Fermi level (at 0 eV), these bands crossings are called Weyl nodes. 2 are represented on the plotted band structure, and TaAs exhibits 24 Weyl nodes in total. The shape of the band structure sketched here is characteristic of Weyl semimetals: bands gaps except in some regions called Weyl nodes. The band structure that we calculated is in good agreement with other first-principles calculations [3].

Phonon dispersion curve



As we can see on the dispersion curve, there is no gap between acoustic and optical modes, but there are two regions of bands. Indeed, Ta atoms contribute mainly at low frequencies and As atoms at high frequencies. Moreover, this dispersion curve exhibits the same shape and frequencies as experimental and theoretical data [1], even if we only used a 4x4x4 q-point grid. The phonon frequencies at Γ (in $cm^{-1} \times 10^2$) are: 0.000 ; 1.178 ; 1.629 ; 2.228 ; 2.412 ; 2.420 ; 2.513.

Electron-phonon coupling and mobilities

In order to compute the electron-phonon coupling and mobility of TaAs, our goal is to solve the linearized Boltzmann Transport Equation (BTE). The results presented in this poster are obtained using the Iterative Boltzmann Transport Equation (IBTE) method [4]. This iterative solving of the BTE, within the EPH module of *Abinit*, allows us to calculate the transport coefficients and, more specifically, the electrical conductivity tensor σ_{ij}. The conductivity is given by: $\sigma = n_e\mu_e + n_h\mu_h$, where n_e and n_h are the electron and hole concentrations in the conduction and valence bands respectively, and μ_e and μ_h are the electron and hole mobilities. The separate contributions of holes and electrons to the conductivity can be taken into account, but here, we do not make the difference between the carriers. They present therefore the same concentrations (calculated at $T = 0K$, $n = 1.92 \times 10^{18} cm^{-3}$), mobilities and conductivities.

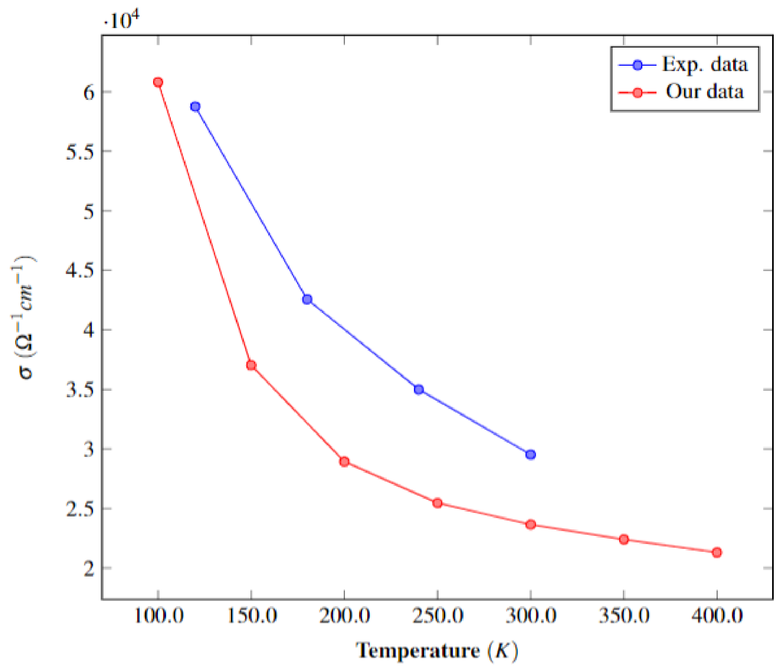


Figure 1: Longitudinal conductivity σ of TaAs w.r.t the temperature, calculated with a 60x60x60 customized k-point grid, 60x60x60 interpolated q-point fine grid and a energy range around the Fermi level of 0.25 eV. The curve in red stands for the data that we calculated, the one in blue stands for experimental data coming from [2].

Temperature (K)	100	150	200	250	300	350	400
μ	9.893	6.027	4.708	4.144	3.849	3.645	3.466

Table 2: Calculated carriers mobility μ (in $m^2V^{-1}s^{-1}$) of TaAs at different temperatures.

Results and discussion

The conductivities calculated are quite close to the experimental ones, underestimating by between 0.5 and 1 $\Omega^{-1}\text{cm}^{-1}$, or about 15%. The results are numerically well converged and they likely describe correctly the reality of transport in TaAs. Calculations at lower temperatures would be interesting because this kind of material exhibits even larger mobilities in the low temperature regime [2]. However we have found that transport properties at low temperatures are more difficult to converge, as the derivative of the Fermi-Dirac distribution is strongly peaked around the Fermi level, making an even denser sampling is needed to converge the Brillouin zone integrals.

Conclusion and perspectives

A full first-principles study (DFT, DFPT and Boltzmann transport) of transport in the Weyl semimetal TaAs has been achieved and presented in this poster and compared with existing literature. The next steps are to calculate the mobilities at low temperatures and calculate other transport coefficients, such as Hall, Nernst and Seebeck coefficients. The full study of TaAs is interesting as a test bed. Once these next steps mentioned above are completed, additional transport terms will be calculated, including the Berry phase contribution to the velocity.

References

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