Layer-dependent Optical Conductivity of MBE-grown $ZrTe_2$

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Besides providing an interesting platform to interrogate fundamental physics questions, two-dimensional transition metal dichalcogenides (TMDCs) are well suited to advance the development of optoelectronic technologies. In this work, we investigated the growth and the optical properties of $ZrTe_2$, a candidate topological Dirac semimetal, grown using molecular beam epitaxy. During the growth of 12 unit cells (u.c.) of $ZrTe_2$ on a sapphire substrate, we obtained in-situ spectroscopic ellipsometry after the deposition of each u.c. Additionally, we obtained temperature dependent ellipsometry data on the sample between 20 °C and 350 °C. After the deposition of the $ZrTe_2$ layers, a Te capping layer was deposited in order to protect the TMDC film. Post-growth X-ray reflectivity measurements indicated that the total thickness of $ZrTe_2$ and the thickness of Te to be 5.95 nm and 19 nm, respectively.

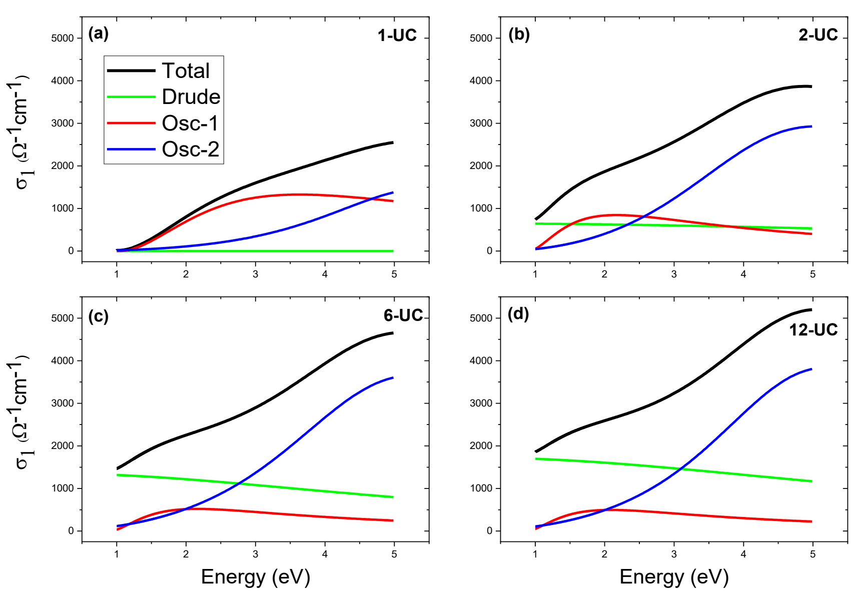

Fig. 1. Total conductivity (black-lines) and contributions from free electrons (green-lines) and band electrons (red and blue lines) for different thicknesses of $ZrTe_2$.

A standard inversion technique was used to model the ellipsometry spectra by specifying a three layer model (i.e., sapphire substrate, $ZrTe_2$ layer and the Te capping layer) to fit the final ellipsometry spectra. The thicknesses obtained from X-ray reflectivity allowed us to obtain the precise dielectric function of the final $ZrTe_2$ layer (i.e., 12 u.c.), which was converted to the optical conductivity. Subsequently, we fit the remaining ellipsometry spectra obtained for 11 u.c. through 1 u.c. $ZrTe_2$ layers. Clearly, the optical conductivity shows a noticeable change with the thickness of the $ZrTe_2$ layers, where the real part increases with the thickness of $ZrTe_2$, as shown in Fig. 1. The layer-dependent conductivity was further analyzed by incorporating a Drude oscillator to account for free electrons, and two Kramers-Kronig-consistent oscillators to represent the band-to-band transitions. Interestingly, we find that the Drude contribution reduces as the thickness of $ZrTe_2$ gets smaller, suggesting that its metallic character diminishes as the thickness reduces.