Towards $PtSe_2$ Intrinsic Properties for High Frequency (Opto)electronics

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$PtSe_2$ is an original transition metal dichalcogenide exhibiting high carrier mobility and thickness dependent electronic properties, transitioning from a semiconductor with a bandgap of ~ 2 eV for 1 monolayer (ML) to a semimetal with zero bandgap for multilayers. We have synthesized $PtSe_2$ multilayers on low cost sapphire substrates by molecular beam epitaxy (MBE) exhibiting high crystalline quality [1], high carrier mobility [2], and high optical absorption at 1.55 µm [3]. With 14MLs-thick $PtSe_2$ film grown on a 2-inch wafer, we demonstrated 60 GHz bandwidth photodetectors and 30 GHz optoelectronic mixers [1].

To achieve the synthesis of highly conductive $PtSe_2$ films, we developed a robust methodology to evaluate film quality using Raman metrics. We demonstrate that the crystalline quality and the transport properties of $PtSe_2$ films can be efficiently monitored by Raman peak widths, considering not only the commonly used E_g full width at half maximum (FWHM) but also the A_{1g} FWHM. Fig. 1 shows a strong correlation between both E_g and A_{1g} FWHMs and sheet conductance for our MBE "Gen1" and "Gen2" films. This correlation was also investigated, when compared to films obtained by thermally assisted conversion [4]. Our in-depth structural analyses, using X-ray diffraction and scanning transmission electron microscopy (STEM), revealed that the A_{1g} FWHM reflects the out-of-plane crystalline quality of multilayer $PtSe_2$ films, which has a significant impact on film conductivity. To investigate the impact of domain arrangement, 4D-STEM structural mapping [5] was carried out, highlighting the critical importance of vertical alignment of superimposed domains in the film thickness for high conductivity. Complementary DFT calculations demonstrated that stacking faults alter the local electronic properties, thereby influencing the overall conductivity of the film. With a highly crystalline $PtSe_2$ film exhibiting E_g and A_{1g} FWHMs of 3.5 cm^{-1}, we achieved a record sheet conductance (1.6mS) compared to grown films, matching the best reported value for exfoliated multilayers. However, exfoliated multilayer $PtSe_2$ with E_g and A_{1g} FWHMs of ~ 2.5 cm^{-1} have been recently obtained [6], and we have grown, by MBE, $PtSe_2$ layers on h-BN flakes with E_g FWHM as low as 2.2 cm^{-1}. Based on the Raman metrics shown in fig. 1, this suggests that the intrinsic properties of this material have not yet been experimentally demonstrated, which seems to confirm the high potential of $PtSe_2$ for electronic and optoelectronic applications.

References

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[3] Tharrault et al., Phys. Rev. Lett. 134, 066901 (2025)
[4] Lukas et al., Adv. Funct. Mater. 2102929 (2021)
[5] Dosenovic et al, 2D Mater. 10 045024 (2023)
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Figures

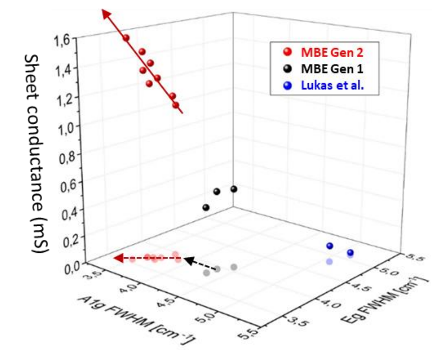

Figure 1 : Sheet conductance of $PtSe_2$ multilayers as a function of E_g and A_{1g} FWHMs

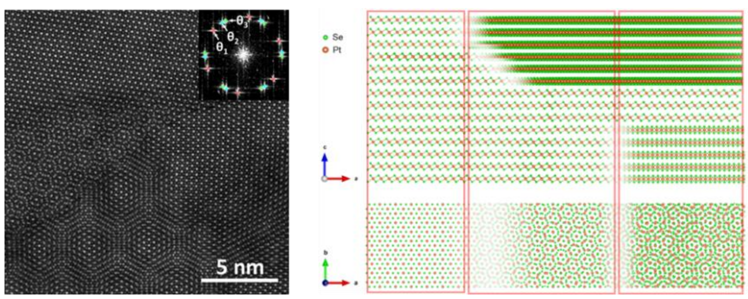

Figure 2: Plan view STEM image of superimposed twisted domains and schematic illustration of typical domain arrangement