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Carrier Trapping by Oxygen Impurities in Molybdenum Diselenide

Abstract
Trapping of photo-excited carriers by oxygen impurities is studied with ultrafast pump-probe spectroscopy. In exfoliated multilayer $MoSe_2$, oxygen impurities are intentionally created with Ar+ plasma irradiation and air exposure. After plasma treatment, the signal of transient absorption shows a signature of defect capturing carriers. (Fig. 1a) In CVD grown monolayer $MoSe_2$, oxygen impurities are induced during the growth process and confirmed with X-ray photoelectron spectroscopy [1]. For both samples, the observed defect state filling shows a clear saturation at high exciton densities, from which the trapping defect densities are estimated from the transient absorption signal. In CVD grown monolayer $MoSe_2$, the defect density is around "$0.5\times10^{12}/cm^2$. The exciton capture time extracted from experimental data is around ~1ps, while the average fast and slow release times are 52ps and 700ps, respectively. In plasma treated exfoliated sample, the trapping defect density increases with plasma irradiation time. (Fig. 1b) First principle calculations with density functional theory reveal that oxygen atoms occupying Mo vacancies create mid-gap defect states, which are responsible for the carrier trapping [2]. However, the occupation of chalcogen vacancies by oxygen atom (Mo-O bonding) can remove the mid-gap state and restore the band structure to a clean defect-free band gap [3]. Our results imply that even the same defect species, e.g. oxygen atoms in this case, can have remarkably different effects on band structure and carrier dynamics in TMDs, depending on their position in the host lattice.

References

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[3] Liu, Y., Stradins, P., and Wei, S.H., 55(3) (2016), 965-968.

Figures

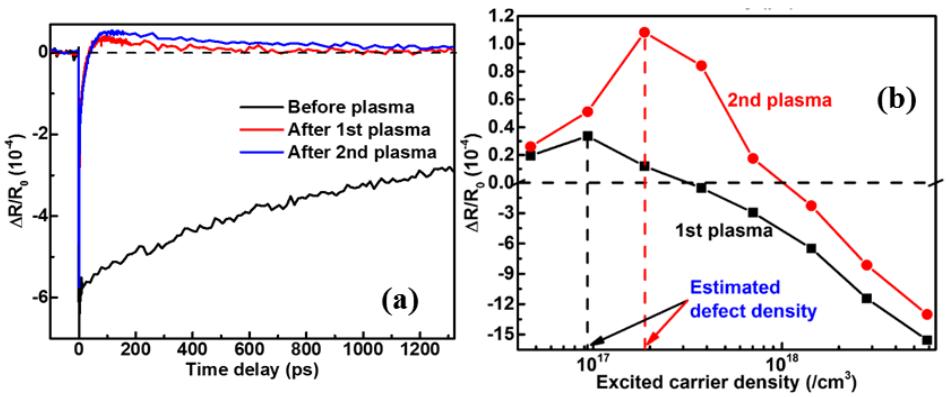

Figure 1: (a) Transient differential reflection signals of exfoliated MoS_2 before and after plasma irradiation. (b) ΔR/R0 values at certain delay times as a function of excited carrier density