Upper Valley and Degeneracy Interplay on the Mobility of Transition Metal Dichalcogenides: Insights from Monte Carlo Simulation

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INTRODUCTION

Carrier mobility and carrier high-field drift velocity of transition metal dichalcogenides (TMDs) are fundamental transport properties needed to advance the TMD device technology. Despite an ongoing research, significant disparities between experimental results and theoretical models persist, largely due to a significant surface-to-volume ratio of atomically thin TMDs, which renders them particularly susceptible to environmental factors.

In this study, we employed our in-house ensemble Monte Carlo (EMC) simulator to examine the impact of degeneracy and screening on a low-field electron mobility and a high-field electron drift velocity, specifically studying the influence of carrier concentration and temperature. We accounted for a full screening of scattering events, including intrinsic processes [1]. Our findings indicate that free carrier screening, along with other factors, plays a crucial role in comprehending the non-monotonic behavior of mobility as a function of carrier concentration in the most widely used TMDs, such as MoS_2 or WS_2.

MODEL

The in-house EMC simulator was successfully tested in previous research on various 2D materials [2-5]. The transport model employed a multi-band, multi-valley band structure, with the conduction band of TMD materials described by primary valleys (K points of the first Brillouin zone) and secondary valleys (Q points) utilizing parabolic dispersion relations in the vicinity of the valley minima. In the valence band, the maxima are situated in the K points, as for direct gap materials, while the secondary valleys are located at the Γ point at lower energy (see Table 1). Effective masses for electrons and holes are derived from density functional theory calculations [6, 7]. Isotropic masses were considered for the K valleys, while longitudinal and transverse effective electron masses are considered for the Q valleys. This analytical description of the bands has demonstrated a good agreement with full-band models in EMC simulations for TMDs, while being more computationally efficient [8].

RESULTS

This study analyzed the effect of free carrier screening and degeneracy on the electronic transport properties of 2D TMD materials supported on a dielectric substrate. The EMC simulator showed that the mobility of electrons and holes exhibited a strong non-monotonic dependence (see Fig. 1) with carrier concentration n at the lowest temperature under study. The highest mobility for electrons was achieved at $T = 77$ K and $n = 5 \cdot 10^{12}$ cm^{-2}. At intermediate n values, the progressive increase in electron mobility up to maximum values is attributed to the effect of screening on intrinsic scattering mechanisms in the K valleys. At larger n, the mobility dropped due to the increasing proportion of electrons reaching the upper Q valleys, leading to additional electron scatterings. The electron drift velocity at high electric fields was influenced by the SPP scattering in the K valleys, acting as an effective energy relaxation mechanism.

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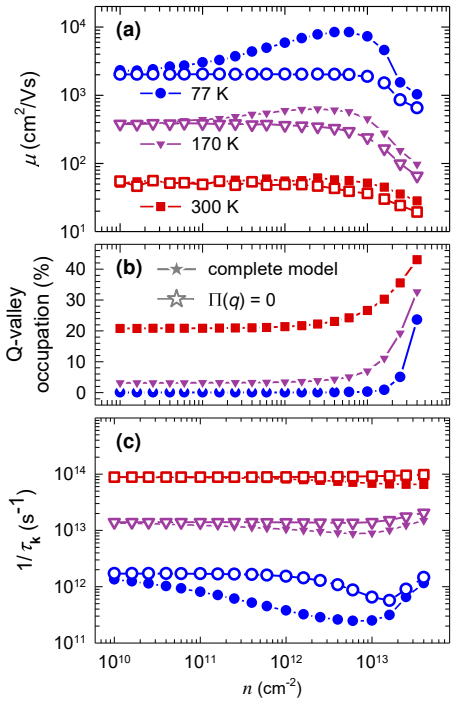

Fig. 1. (a) Low-field electron mobility, (b) upper (Q) valley occupation, and (c) inverse of momentum relaxation time due to scattering mechanisms at three different temperatures in monolayer MoS_2 supported on a SiO_2 substrate. Solid symbols relate to simulations accounting for all the phenomena of the EMC model, and open symbols to results where the screenings due to free carrier is omitted.

	Conduction band			Valence band		
TMD	m^*_K (u. of m_0)	$m^*_{Q,\parallel}, m^*_{Q,\perp}$ (u. of m_0)	$\varepsilon_{0,Q} - \varepsilon_{0,K}$ (meV)	m^*_K (u. of m_0)	m^*_Γ, (u. of m_0)	$\varepsilon_{0,K} - \varepsilon_{0,\Gamma}$ (meV)
MoS_2	0.50	0.62, 1.00	70	0.58	4.05	148
WS_2	0.31	0.60, 0.60	67	0.42	4.07	173
$MoSe_2$	0.64	0.80, 0.80	28	0.71	7.76	374
WSe_2	0.39	0.64, 0.64	16	0.51	7.77	427

Table 1. Band structure parameters for the effective mass approximation in various TMDs.