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How high can the mobility of monolayer tungsten disulfide be?

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ABSTRACT

Monolayer tungsten disulfide is a very promising two-dimensional material for future transistor technology. Monolayer tungsten disulfide, owing to the unique electronic properties of its atomically thin two-dimensional layered structure, can be made into a high-performance transistor device. In this paper, we focus on band-structure and carrier mobility calculations for monolayer tungsten disulfide. We use the tight-binding (TB) method and modified effective mass approximation (MEMA) to calculate the band-structure, density of states, velocity square, and other physical quantities of monolayer tungsten disulfide. Electron mobility using the Kubo–Greenwood formula is calculated based on the TB and MEMA band model, respectively. The phonon-limited electron mobility of monolayer can be reached to ~700 cm^2/Vs. Our results help to design the future nanoelectronic devices with monolayer WS_2.

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1. Introduction

A two-dimensional material is a candidate channel material for an ultra-thin-body transistor device, owing to its perfect electrostatic control. Graphene is the most common two-dimensional material with a high mobility but no band-gap. Even film materials with one or several layers of atoms have become candidate two-dimensional material for future transistor technology. Among two-dimensional materials, graphene, boron nitride (BN), and transition metal dichalcogenide (TMD) are particular areas of focus. Unlike graphene and BN, TMD such as WS_2 is a semiconductor. The WS_2 layer structure exhibits similar performance to graphite, such that WS_2 could be used for a high performance transistor device. Tungsten disulfide (WS_2), with its two-dimensional super-thin atomic structure and unique optical and electronic properties, has been broadly studied in past years. According to the previous simulation work of the research team from UC Berkeley [1], owing to the heavier electron effective mass and a lower mobility, monolayer MoS2 is not the best option for high performance transistor device. It is necessary to find other TMD materials with larger electron mobility. The best mobility can be achieved is limited by the intrinsic scattering. Phonon scattering is the one which cannot be avoided at temperatures other than zero. There are quite a few works aimed to calculate the phonon-limited electron mobility in monolayer TMD materials. The electron mobility calculation for monolayer MoS2 was reported by Dr. Kaasbjerg's research group [2]. The calculated room temperature mobility of monolayer MoS2 is about 400 cm^2/Vs which sets the upper bound of electron mobility. Very recently, Prof. Kim's research group from North Carolina State University [3] calculated the phonon limited electron mobility of four typical monolayer TMDs including MoS2, MoSe2, WS2 and WSe2. Monolayer WS2 provides the best performances of electron with high mobility among these four typical TMD materials. Prof. Zhang's research team calculated the electron mobility for 14 TMD materials and approximated the electron phonon scattering matrix by deformation potentials, within which long wave longitudinal acoustical and optical phonon scatterings were included [4,5]. They found that out of the 14 compounds, monolayer WS_2 is a promising option for logical devices regarding the possible high electron mobility and finite band-gap.

Recently, Prof. Esseni's research group from Udine University [6] developed the method to calculate the electron mobility based on Kubo-Greenwood mobility formula and obtained similar results. Prof. Jing Guo's research group [7] reported that the performance limits of monolayer TMD transistors are examined with a ballistic MOSFET model. Using an *ab initio* theory, they calculated the band-structures of typical monolayer TMD. They found within the ballistic regime, the performances of monolayer WS_2 transistor is better compared with those of the silicon transistors if a thin high-κ gate insulator is used. This makes monolayer WS_2 a promising 2-D material for future nano-electronic device applications.

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In this work, the band-structure and electron mobility of monolayer WS_2 as a potential channel material in future transistor devices are studied. In sections 2, calculation method for band-structure models and electron mobility of monolayer WS_2 are presented. The results of the study are discussed in section 3. Section 4 presents a summary of this study.

2. Calculation method

Kubo–Greenwood Mobility Formula [6], 8–12] is shown as following.

$$\mu_{xx} = \frac{e\int_{E0}^{\infty} D(E)V_x^2(E)\tau_{tot}(E)f(E)[1-f(E)]dE}{kBT\int_{E0}^{\infty} D(E)f(E)dE} \tag{1}$$

$$D(E) = \frac{1}{(2\pi)^2}\int_{BZ} d^2\vec{k}\,\delta\left(E - E\left(\vec{k}\right)\right) \tag{2}$$

$$V_x{}^2(E) = \frac{\left(1/(2\pi)^2\right)\int_{BZ} d^2\vec{k}\,V_x{}^2\left(\vec{k}\right)\delta\left(E-E\left(\vec{k}\right)\right)}{\left(1/(2\pi)^2\right)\int_{BZ} d^2\vec{k}\,\delta\left(E-E\left(\vec{k}\right)\right)} \tag{3}$$

In Eq. (1), f(E) denotes the Fermi–Dirac function, E is the total energy, V_x(E) is the energy-dependent group velocity [8], τ_{tot}(E) is the scattering time, and D(E) is density of states (DOS) [8]. The function D(E) is calculated by following the linear tetrahedron method, which provides a detailed integration over the two-dimensional Brillouin zone. The expression for the x component of the square of the group velocity square averaged over an equi-energetic surface is V_x^2(E), as shown in the denominator of Eq. (3), where $V(\vec{k}) = (\nabla_{\vec{k}}E(\vec{k}))/\hbar$ denotes the group velocity and x is the direction. As a consequence, the total scattering rate, $1/\tau_{tot}$(E), and the contributions from the different coupling types have been obtained using Matthiessen's rule by summing the scattering rates from the individual phonons,

$$\frac{1}{\tau_{tot}(E)} = \frac{1}{\tau_{ADP}(E)} + \frac{1}{\tau_{ODP}(E)} + \frac{1}{\tau_{PLO}(E)} \tag{4}$$

The scattering rate on acoustic phonons is given by

$$\frac{1}{\tau_{ADP}(E)} = \frac{2\pi}{\hbar}\left[\frac{D_{AC}^2 K_B T}{\rho v_s{}^2}\right]D(E) \tag{5}$$

The scattering rate on optical phonons is given by

$$\frac{1}{\tau_{ODP}(E)} = \frac{2\pi}{\hbar}\left[\frac{\hbar^2 D_{OP}^2}{2\rho\omega_{OP}}\right]\left[N_q D(E) + (N_q+1)D(E-\hbar\omega_{OP})\Theta(E-\hbar\omega_{OP})\right]$$

$$N_q = \frac{1}{e^{\frac{\hbar\omega_{OP}}{K_B T}} - 1} \tag{6}$$

where N_q is Born-Einstein distribution.

In monolayer WS_2, the polarization from the lattice vibration of the polar LO phonon is oriented along the plane of the layer. Using microscopic approach based on the atomic Born effective charges, a scattering rate formula, τ_{PLO}(E), for the polar LO phonon interaction in monolayer WS_2 is followed by Ref. [6] and not presented here.

In the present study, the band-structure of monolayer WS_2 is calculated with three band tight-binding model [13,14] reported by Ref. [13]. As you can see in Fig. 1, the conduction band is perfectly parabolic in the K valley in small energy region. Due to their isotropic and parabolic effect in small energy region, the part of the conduction band relevant for the electron mobility can to a good approximation be described by effective mass approximation (EMA) band as reported from Ref. [14]:

$$E = \frac{\hbar^2\left(k_x{}^2 + k_y{}^2\right)}{2m^*} \tag{7}$$

Recently, Prof. David Esseni's research group [6] proposed the first order modified EMA (MEMA 1st) conduction band model only considering non-parabolicity fasctors, α as shown below.

$$E(1+\alpha E) = \frac{\hbar^2\left(k_x{}^2 + k_y{}^2\right)}{2m^*} \tag{8}$$

In this work, we proposed modified EMA (MEMA) model considering two non-parabolicity factors, α and β. Assuming a non-parabolic dispersion relation is presented as below.

$$E\left(1+\alpha E+\beta E^2\right) = \frac{\hbar^2\left(k_x{}^2 + k_y{}^2\right)}{2m^*} \tag{9}$$

Note that the non-parabolicity factors, α and β, are extracted from the TB-calculated electronic band-structure.

3. Discussion and results

Fig. 1 presents the result using a three band tight-binding (TB) model, where the band at the degeneracy of K and K′ can be observed, with the direct band-gap. Result from MEMA conduction band model is also included for comparison. The band-structure acquired from a three band tight-binding model is further used for calculating the DOS, as shown in Fig. 2, where the energy shown in the figure is up to 250 meV. Comparison of DOS of the TB band model (symbol), EMA (green line), MEMA 1st (blue line), and MEMA model (red line) for monolayer WS_2 is also included. Inset

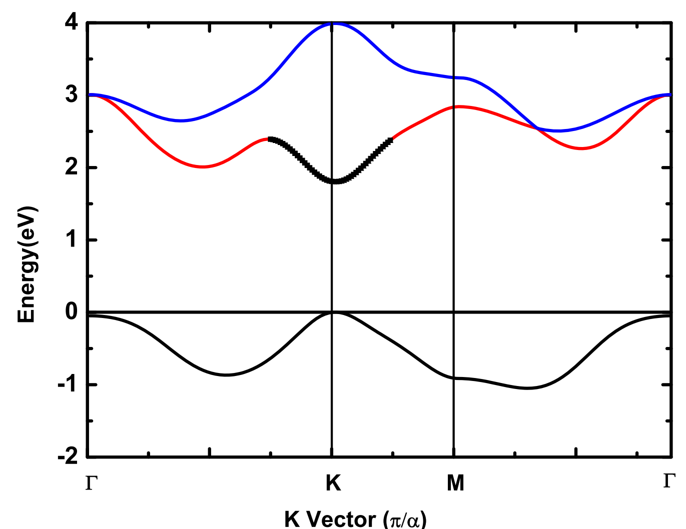

Fig. 1. Calculation of the band-structure of monolayer WS_2 with a three-band TB model. MEMA conduction band model (black square dots) is also included for comparison. The x-axis is K vector in the in-plane Brillouin zone which characterized by high-symmetry points Γ=(0, 0), K = 4π/3a (1, 0), and M = 4π/3a (0, $\sqrt{3}/2$). Note that a is lattice constant of monolayer WS_2.

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