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Comparative Simulation Study of Intra-Layer Band-to-Band Tunneling in Monolayer Transition Metal Dichalcogenides

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Inter-layer band-to-band tunneling through monolayer transition metal dichalcogenides is calculated by using the nonequilibrium Green function method. Material depdence of the transmission function $T(E)$ is shown to be basically understood in terms of the tunneling masses. $T(E)$ of a nanoribbon structure is found to decay rapidly with the tunneling distance compared with that of the corresponding bulk system.

1 Introduction

Transition metal dichalcogenides (TMDCs) have potential for application of nano-devices because of their unique physical and electrical properties [1]. Recently, tunnel field-effect transistors utilizing band-to-band (BTB) tunneling in TMDC were fabricated, showing excellent device characteristics [2]. In the previous study [3], we have performed a comparative study on the inter-layer BTB tunneling in vdW junctions consisting of various TMDC layers by using non-equilibrium Green function (NEGF) method combined with a tight-binding (TB) approximation. In the present study, we have studied intra-layer BTB tunneling in various monolalyer TMDCs by using the TB-NEGF method. We especially focus on difference between the BTB tunnel transmission function of a nanoribbon structure and that of the corresponding bulk system.

2 Calculation model and method

We consider bulk TMDCs of WTe_2, WS_2, WSe_2, $MoTe_2$, MoS_2, and $MoSe_2$, and zigzag-edge nanoribbon structures. The schematic diagram of the nanoribbon structure is given in Fig. 1. The nanoribbon has infinite length along the x-direction and finite width along the y-direction. The edge of the nanoribbon is terminated by hydrogen atoms.

We use 11-band TB model [4] whose parameters are extracted from a density functional theory (DFT). Figures 2 and 3 show the band structure of bulk MoS_2 and nanoribbon MoS_2, respectively. The TB band-structure shows a good agreement with the DFT band-structure, especially near the band edges. The transmission function, $T(E)$, is calculated by the NEGF method with applying the Eckart potential [5] to the system. The bottom of the conduction band of the right electrode is set to 0 eV and the top of the valence band of the left electrode is set to ΔE. We define the tunneling distance ℓ as the spatial distance between the conduction and valence band edges at $E = \Delta E/2$ (see Fig. 1).

3 Results and discussion

Figure 4 shows $T(E)$ as a function of ℓ for bulk TMDCs. The transmission function exponentially decreases with ℓ. We see that the BTB tunneling of materials consisting of W-atom becomes larger than that of Mo-atom. As shown in Fig. 4, the decay rate is basically understood in terms of the tunneling mass $m_t = (m_c^{-1} + m_v^{-1})^{-1}$ where m_c and m_v are the band-edge mass of the conduction and valence bands, respectively. Figure 5 shows $T(E)$ for MoS_2 and WS_2 nanoribbons. We find that $T(E)$ of the nanoribbons decay rapidly compared with that of the bulk system (see Fig. 6). Although the band-edge masses are heavier in the nanoribbons, this difference cannot be explained solely in terms of the difference in the tunneling mass. The electronic states of the top two valence bands are localized near the nanoribbon edges, which may cause the difference. We also find small structures appearing on the ℓ-dependence of $T(E)$ as indicated by arrows in Fig. 5. This may be originated in quantum interference between the band edges.

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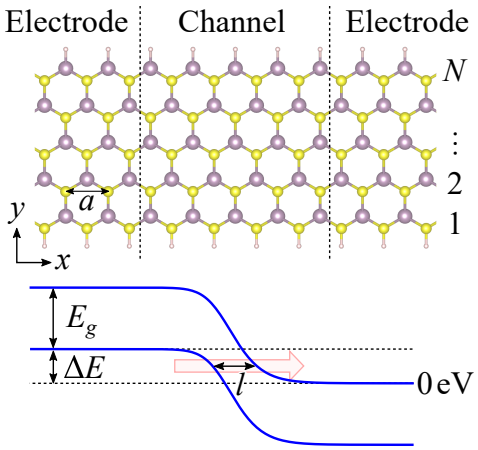

Fig. 1: Schematics of the zigzag-edge nanoribbon structure (top) and the band profile (bottom).

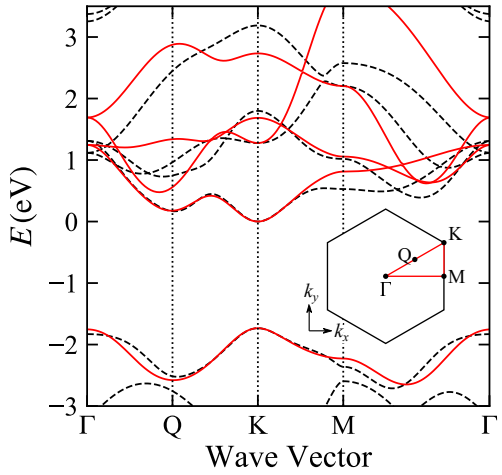

Fig. 2: Band-structure of bulk MoS_2 calculated by DFT (dashed line) and TB method (solid line). Inset shows the first Brillouin zone.

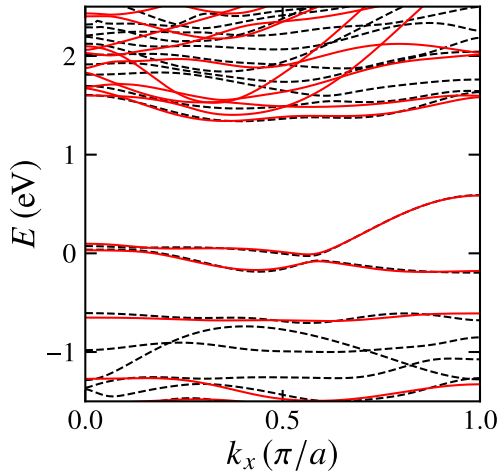

Fig. 3: Band-structure of MoS_2 nanoribbon calculated by DFT (dashed line) and TB method (solid line) for $N = 5$.

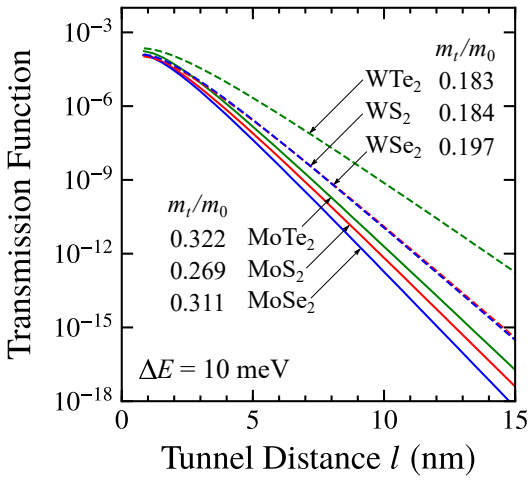

Fig. 4: ℓ-dependence of $T(E)$ of bulk TMDCs at $E = \Delta E/2$ for $\Delta E = 10$ meV.

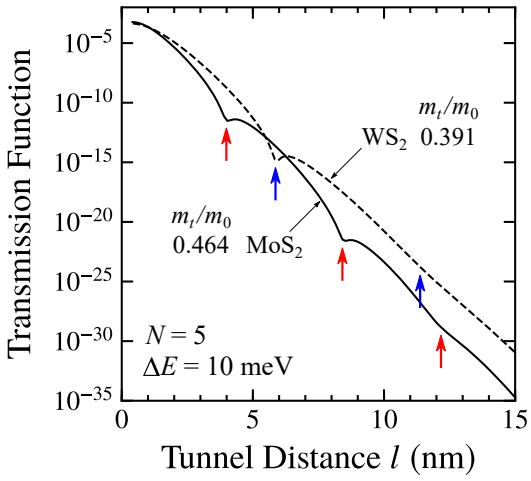

Fig. 5: The same as Fig. 4 but for the nanoribbon MoS_2 (solid line) and WS_2 (dashed line) for $N = 5$.

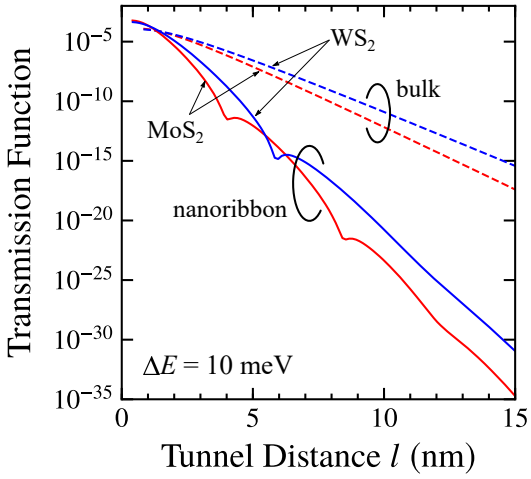

Fig. 6: Comparison between bulk $T(E)$ (dashed lines) and nanoribbon $T(E)$ (solid lines) at $E = \Delta E/2$ for $\Delta E = 10$ meV.