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Resonant Enhancement of Band-to-band Tuneling in In-plane MoS_2/WS_2 Heterojunctions

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Abstract

Band-to-band (BTB) tunneling current through MoS_2/WS_2 in-plane heterojunctions is calculated by using the nonequilibrium Green function method. For the type-A heterojunction with a potential notch at the heterointerface, a resonant enhancement of BTB tunneling leads to significantly larger BTB current compared to the type-B structure without a potential notch.

1 Introduction

Transition metal dichalcogenide (TMDC), such as MoS_2 and WS_2, has been attracted much attention for use in electronic devices. Recently, in-plane TMDC heterojunctions were fabricated [1, 2], which provide an efficient means of studying and optimizing the electrical properties for future device applications such as tunnel field-effect transistors (TFET) [3]. For MoS_2/WS_2 in-plane heterojunctions, two kinds of band profiles can be considered depending on the relationship between the band edge and the applied potential profiles. Figure 1(a) shows the type-A band profile in which a potential notch appears at the heterointerface, while no potential notch for the type-B (see Fig. 1(b)). In the previous study [4], we reported that for type-A MoS_2/WS_2 in-plane heterojunctions the band-to-band (BTB) tunneling is enhanced when the electrons tunnel through virtual bound states associated with the potential notch. In the present study, we have performed a comparative study of the BTB tunneling through MoS_2/WS_2 in-plane heterojunctions between type-A and type-B structures.

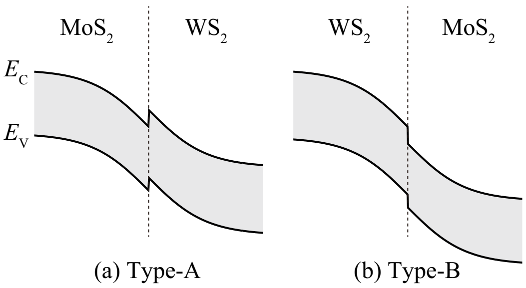

Fig. 1: Two kinds of band profiles for MoS_2/WS_2 in-plane heterojunctions. (a) Type-A band profile has a potential notch at the heterointerface, while (b) type-B has no potential notch.

2 Theory

We calculate the BTB tunneling characteristics using the nonequilibrium Green function (NEGF) method combined with a tight-binding (TB) approximation. We first extracted the TB parameters describing the bandstructure of MoS_2 and that of WS_2 from first-principles calculations. We used the VASP code with the HSE06 functional employed for both exchange and correlation. For the TB approximation, we adopted the three band TB model of Liu *et al.* [5]. The TB parameters at a heterointerface were determined by the arithmetic mean of the parameters on both sides of the interface. For the band discontinuity at the interface, we used the reported values of Ref. [3]. The transmission function, $T(E)$, is calculate by the NEGF method with applying the Eckart potential $U(x)$ [6] to the system. The applied potential has two geometrical parameters: characteristic length, L and the separation between the center position of the potential and the heterointerface, Δy.

3 Results and discussion

Figures 2 and 3 show the band-edge profiles, $U(x)$, and $T(E)$ for type-A and type-B MoS_2/WS_2 heterojunctions, respectively. The BTB tunnel current flows in the energy region of width $\Delta E = 0.3$ eV where the left valence-band and the right conduction-band overlap each other.

To estimate the BTB tunneling current, we define the integrated transmission function, J, by $J = \int T(E)\, dE$, which is proportional to the maximum BTB tunneling current. Figure 4 shows Δy dependence of J of type-A and type-B MoS_2/WS_2 heterojunctions. In Fig. 4, we also plotted J of MoS_2 and WS_2 homojunctions for comparison. We see that J of the heterojunctions can be greater than J of the homojunctions. J of type-A MoS_2/WS_2 heterojunction exhibits oscillatory changes as a function of Δy. This originates in the resonant transmission through virtual bound states associated with the

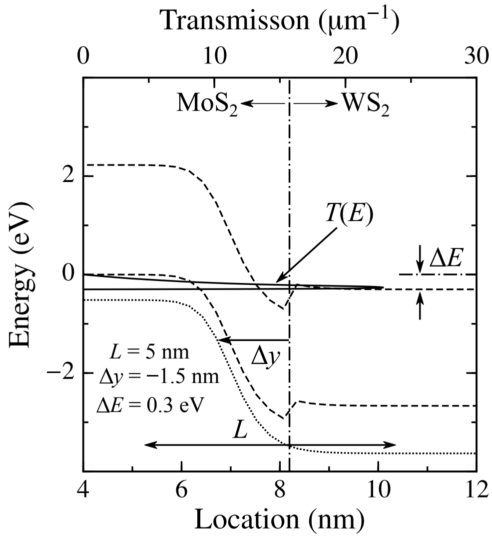

Fig. 2: Band-edge profiles (dashed lines) and transmission function, $T(E)$, (solid line) for the type-A MoS_2/WS_2 heteroj unction. Dotted line shows the applied potential profile (vertically shifted for clarity).

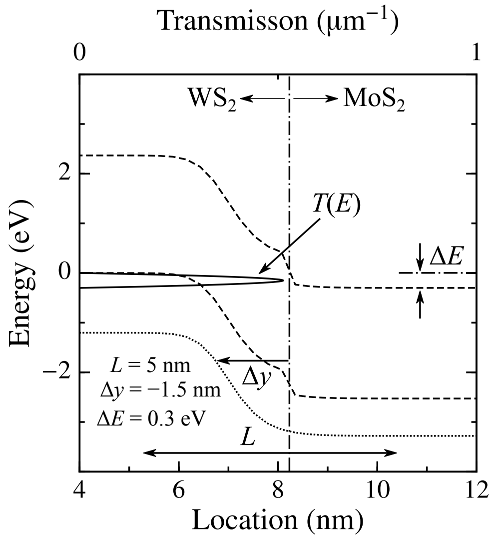

Fig. 3: The same as Fig. 2 but for the type-B heterojunction.

potential notch [4]. Because of the resonance, J of the type-A structure is strongly enhanced and becomes significantly larger than J of the type-B structure.

Figure 5 shows L dependence of J. Note that for the heterojunctions Δy is adjusted to obtain the maximum J for each L. We find that J decreases exponentially as L increases, and J of the type-A MoS_2/WS_2 heterojunction is strongly enhanced compared to the type-B structure.

4 Conclusion

In this study, we calculated J of type-A and type-B MoS_2/WS_2 heterojunctions using the NEGF method,

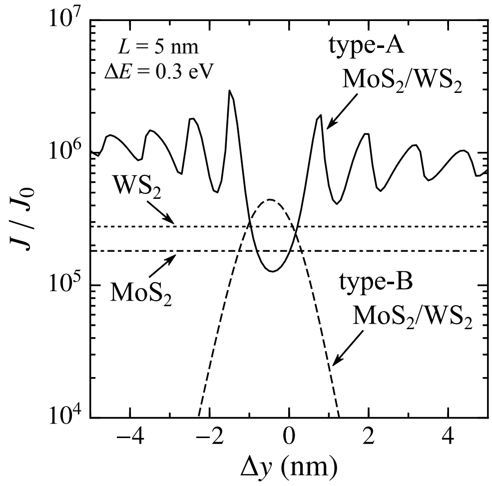

Fig. 4: Δy dependence of J of type-A and type-B MoS_2/WS_2 heterojunctions compared with MoS_2 and WS_2 homojunctions.

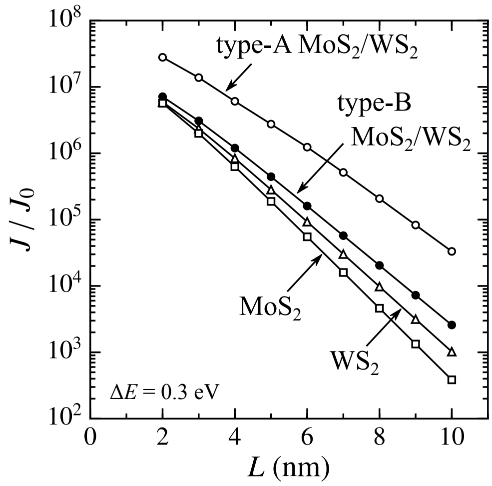

Fig. 5: L dependence of J of type-A and type-B MoS_2/WS_2 heterojunctions compared with MoS_2 and WS_2 homojunctions.

and analyzed the BTB tunneling characteristics. We have shown that both type-A and type-B MoS_2/WS_2 heterojunctions are able to support large J compared to MoS_2 and WS_2 homojunctions. We find that the resonant enhancement of J in the type-A heterojunction leads to significantly larger BTB current compared to the type-B structure.

References

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