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Theoretical Study on Thermoelectric Properties of Ge and Si Nanowires

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1. Introduction

Advanced thermoelectric materials have received considerable attention due to the increasing demand on sustainable energy solution. It was proposed that nanostructures could enhance the thermoelectric performance [1], which is measured by the dimensionless figure of merit, $ZT = S^2\sigma T/\kappa$, where S, σ, T and κ are the Seebeck coefficient, electrical conductivity, absolute temperature and thermal conductivity, respectively [2]. In order to obtain high ZT, S and σ in the numerator must be high and κ must be suppressed. Several groups have already demonstrated that thermal conductivity can be greatly reduced by using nanostructures [3, 4]. In this work, the Seebeck coefficient and power factor ($pf = S^2G$, *where G is the electrical conductance*) of Si and Ge Nanowires (NWs) are investigated. The theoretical study and simulation are based on a semi-classical approach under ballistic transport. In order to capture electronic properties in the nano-scale, a $sp^3d^5s^*$ tight-binding model [5] is used to calculate the E-k dispersion relation of Si and Ge NWs with different cross-section sizes (1, 2, 3, 5, and 8nm), shapes (circle, square and equilateral triangle), and orientations (<100>, <110>, and <111>) under n- and p-type doping. We found that thermoelectric properties significantly depend on the size and orientations, whereas shape has little impact as cross-section area and orientation are fixed.

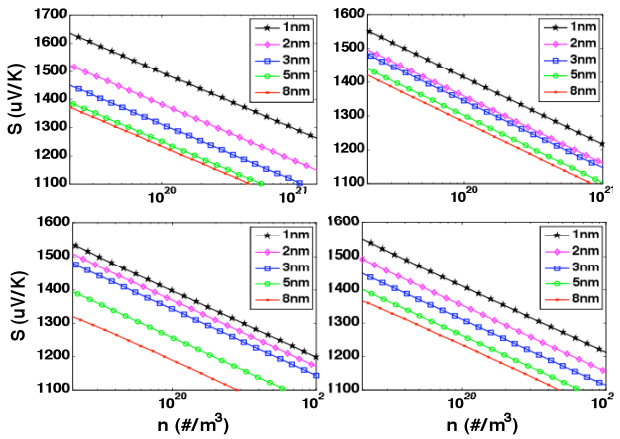


Fig. 1 The Seebeck Coefficient for Si (top) and Ge (bottom) with circle cross-section and <100> orientation of n-type (left) or p-type (right) doping.

2. Results

Figure 1 shows the simulated result of the Seebeck coefficient as function of carrier concentration per volume for n- and p-type Si/Ge NW with <100> orientation with circular cross-section under room temperature. It can be observed that S decreases as the carrier concentration increases. Moreover, S increases as the NW diameter decreases under same carrier concentration. The reasons can be attributed to the increase of carrier effective mass causing by the strong quantum confinement effects for the nano-scale materials. For power factor as shown in Fig. 2, it shows that the first peak value of power factor per area (pf/a) increases as the diameter decreases because the carrier conductivity per area increases as diameter decreases. It indicates that the smaller diameter NWs is more efficient on applications of thermal power devices.

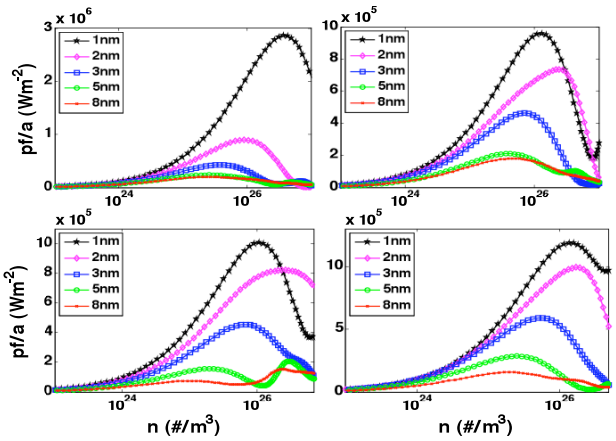
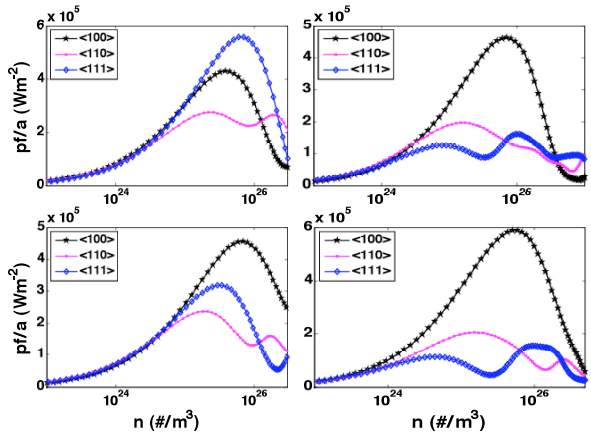


Fig. 2 The power factor for Si (top) and Ge (bottom) with circle cross-section and <100> orientation of n-type (left) or p-type (right) doping.



ig. 3 The power factor for Si (top) and Ge (bottom) with 3nm iameter and circle cross-section of n-type (left) or p-type (right) oping.

Next, we investigate the effect of orientation for 3nm circle Si and Ge NWs as shown in Fig. 3. For all different combinations, the first peak values for pf/a have the same order from highest to lowest. For

n-type doping, the order is <111>, <100>, <110> for Si NWs and <100>, <111>, <110> for Ge NWs; while for p-type it is <100>, <110>, <111> for both Si and Ge NWs (Fig. 3). Therefore, it shows that orientation plays an important role in the thermoelectric properties of nanowires. The reasons of the order of the peak values are due to the different carrier effective mass (m^*) along these orientations, cf., Fig. 4. At a fixed carrier concentration, in general, S is proportional to m^* and G is inversely proportional to m^*. Therefore, power factor (S^2G) should be proportional to m^*. It is shown that the corresponding orders of m^*/m_0 is the same as the pf/a for Si/Ge NW of n/p-doping. This also explains why S decreases as the diameter increases as we investigated in Fig. 1.

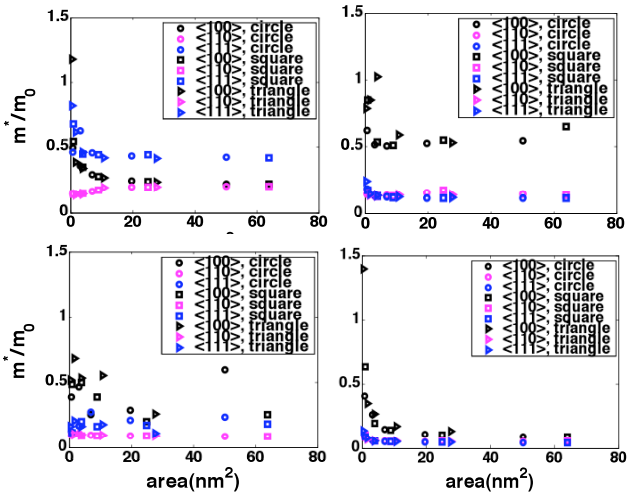
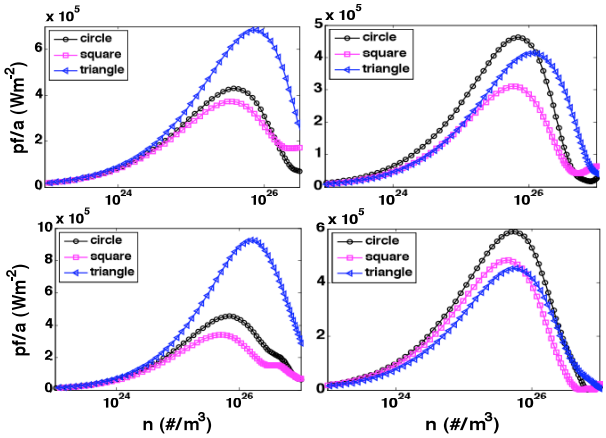


Fig. 4 The effective mass of different carrier concentrations for Si (top) and Ge (bottom) of n-type (left) or p-type (right) doping.



ig. 5 The power factor for Si (top) and Ge (bottom) with 3nm iameter cross-section and <100> orientation of n-type (left) or -type (right) doping.

Fig. 5 shows power factor per area as function of carrier concentration per volume for n- and p-type Si/Ge NW with <100> orientation and 3nm diameter. It can be observed that pf/a varies as shape is changing. However, if we consider pf/a for same cross-section area instead of diameter, we found that pf/a is same for different NW shapes (Fig. 6). The maximum values of pf/a of the first peak are taken from the results under different parameter combinations. Take a close look at pf/a value of <110> direction (blue) at about 10nm², we can see that they are almost same for all shapes.

Furthermore, Fig. 6 also presents that pf/a is significantly increased as the cross-section area decreases to 5nm². For smaller size NWs, <111> shows the best result for n-doped Si NW and <100> shows the best result for p-doped Si NW and n/p-doped Ge NWs in general. From the view of different types of doping, for n-type, Si NWs outperform Ge NWs while for p-type Ge NWs outperform Si NWs. From the view of different materials, n-type is better than p-type for Si, while p-type is better than n-type for Ge.

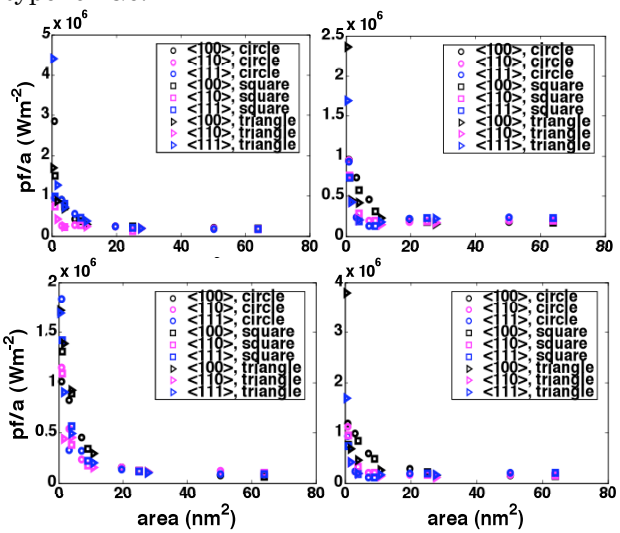


Fig. 6 The maximum power factor of different carrier concentrations for Si (top) and Ge (bottom) of n-type (left) or p-type (right) doping.

3. Conclusions

In summary, we have studied the thermoelectric properties of Si and Ge NWs in terms of Seebeck coefficient and power factor. These thermoelectric performances of Si and Ge NWs are evaluated for different combination of parameters, cross-section sizes, shapes and orientations. The simulation results show that as the nanowire size is decreasing, the performance is greatly improved. Moreover, cross-section orientation and size have the great impact on the results. As other work have shown that NW thermal conductivity could be reduced [5, 6], and to combine that power factor is increased in the NWs, therefore, ZT can be greatly enhanced by using NWs with proper doping and right selection of orientation.

Acknowledgements

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References

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