研究重摻雜矽奈米線之熱電功率因子

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摘　要

研究不同高摻雜濃度(1×10^{19} cm^{-3} ~ 1×10^{20} cm^{-3})矽奈米線之熱電功率因子。首先探討高摻雜濃度 $>4\times10^{19}$ cm^{-3}之下，這矽奈米線之熱電動勢會隨載子濃度增加而下降，換言之，此矽奈米線之熱電動勢結果不受高摻雜雜質的能帶有所影響，接著對於1×10^{19} cm^{-3} < 濃度 < 4×10^{19} cm^{-3}之下，其聲子引曳現象會明顯增加熱電動勢，以致於可以獲得一個最佳的矽奈米線功率因子，因此對於我們研究的矽奈米線元件，這最佳的熱電功率因子是在適當的摻雜濃度 ~2×10^{19}cm^{-3}的矽奈米線。

關鍵詞：熱電，矽奈米線，熱電動勢，聲子引曳

The study of thermoelectric power factor for heavily doped silicon nanowires

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ABSTRACT

Thermoelectric power factor for silicon nanowires, which are heavily doped with carriers having concentrations in the range of 1×10^{19} cm^{-3} to 1×10^{20} cm^{-3}, is investigated. When the carrier concentration is greater than 4×10^{19} cm^{-3}, the Seebeck coefficient (S) decreases with an increase in the carrier concentration; this implies that the influence of an impurity band is negligible. For carrier concentrations less than 4×10^{19} cm^{-3}, the S value increases and the electrical conductivity decreases compared to the values calculated for bulk silicon; this suggests the contribution of phonon drag to the S. For the maximum thermoelectric power, the carrier concentration is approximately 2×10^{19} cm^{-3}.

Key Words: Thermoelectric, silicon nanowires, Seebeck coefficient, phonon drag

I、Introduction

Thermoelectric (TE) devices have attracted much attention because of their ability to produce electricity or electric power from waste heat.[1] Conversion efficiency of TE devices is expressed by the dimensionless TE figure of merit:

$$ZT = \frac{S^2\sigma}{k}T,\qquad(1)$$

where S, σ, k, and T are the thermopower (also called the

Seebeck coefficient), electrical conductivity, thermal conductivity, and operating temperature, respectively. Therefore, ZT can be enhanced by either increasing the power factor (PF), where PF = $S^2\sigma$, or by decreasing the thermal conductivity, k. Maximum effort has been focused on reducing k by alloying,[2] surface roughening,[3] or using nanostructured TE materials.[4] Recently, silicon nanostructures have emerged as promising TE materials due to a significant reduction in their k values compared to that of the bulk silicon;[5,6] the reported k values for the nanostructures are as low as 1~2 $Wm^{-1}K^{-1}$. The PF has become another important index for maximizing TE performance and it can characterize the electric power output.[7] Recent experimental measurements in a heavily doped silicon nanostructure showed an increase in S, which could be attributed to the influence of an impurity band.[8] In another case, the enhanced S value of the heavily doped silicon nanowires (SiNWs) was explained by the effect of phonon drag.[6] Although some studies on the origin of S enhancement have been reported,[6-8] the theoretical analysis is not clearly understood till date. To further improve the performance of the TE device, the PF for the heavily doped SiNWs must be also discussed.

This study focused on the re-examination of the thermoelectric PF for heavily doped SiNWs. Based on the measurements to determine the dependence of S and σ on carrier concentration, the physical understanding of the two parameters, S and σ, in heavily doped SiNWs was substantially improved. In addition, the carrier concentration for maximizing the PF was optimized.

II、Experiments

The top-down SiNWs were fabricated using a CMOS-compatible process with (100) SOI wafers as starting substrates. In this process, SiNWs with a width-to-length ratio of 50 nm / 2 μm were lithographically defined on the SOI wafers with a 50 nm top layer of silicon and 150 nm layer of buried oxide. The SiNW pattern was defined by electron-beam lithography and followed by reactive ion etching. Subsequently, the n-type SiNWs were doped by implanting phosphorous

impurities. The carrier concentration, ranging from 1×10^{19} cm^{-3} to 1×10^{20} cm^{-3}, was confirmed by a homemade Hall measurement system. For the contact regions, a second implantation was done with phosphorous impurities having concentration of approximately 1×10^{20} cm^{-3} to reduce the contact resistance. After the n-type impurities were activated by rapid thermal processing at 1050 ^{o}C for around 30 s, an AlSi layer was deposited to provide connection pads for the electrical and temperature measurements. The S value was determined by the ratio of the thermovoltage (ΔV) to the temperature difference (ΔT), i.e., S=ΔV/ΔT. Two K-type thermocouples were directly attached to the connection pads for the ΔT measurement. The ΔT was generated by two resistive heaters beneath the SiNWs. The time evolution of the ΔV induced by the ΔT was measured using a Keithley 2400 source meter. The σ value was determined from the slope of the current versus voltage curve of SiNWs.

III、Results and Discussion

Figure 1 shows ΔV-ΔT characteristics for SiNWs with various carrier concentrations ranging from 1×10^{19} cm^{-3} to 1×10^{20} cm^{-3}. The value of S was extracted from a linear fit of ΔV versus ΔT. In general, the S value is regarded as the sum of the contributions from the carrier component (S_c) and the phonon component (S_{ph}), i.e. $S = S_c + S_{ph}$. Firstly, when the carrier concentration was greater than 4×10^{19} cm^{-3}, the S_{ph} was assumed to be negligible due to a smaller mean free path of the phonons.[9]
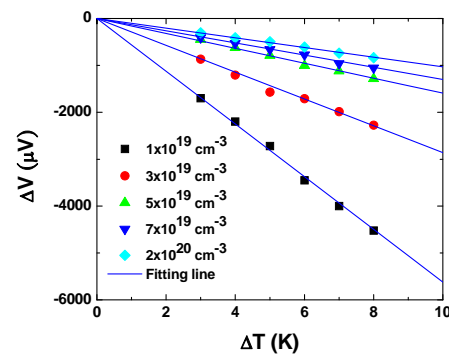

Fig.1 ΔV-ΔT characteristics for SiNWs.

Figure 2 shows that the absolute values of the measured S decreased with an increase in the carrier concentration. For heavily doped SiNWs, the Sc can be estimated using the Mott formula:[10]

$$S_c = \frac{\pi^2 k_B^2}{3q} T \left\{ \frac{d[\ln(\sigma(E))]}{dE} \right\}_{E=E_F}$$

$$= \frac{\pi^2 k_B^2}{3q} T \left\{ \frac{1}{n} \frac{dn(E)}{dE} + \frac{1}{\mu} \frac{d\mu(E)}{dE} \right\}_{E=E_F}$$

$$(2)$$

where k_B and E_F are the Boltzmann constant and the Fermi energy, respectively. Here, the $\sigma(E)$ denotes $n(E)q\mu(E)$, i.e. $\sigma(E) = n(E)q\mu(E)$, with n representing the carrier density and μ representing mobility. However, without considering the scattering factor, neglecting the second item of Eq. (2), S_c is further approximated as

$$S_c \approx \frac{8\pi^2 k_B^2}{3qh^2} m^* T \left(\frac{\pi}{3n} \right)^{2/3} \qquad (3)$$

with the density of states

$$g(E) = \frac{(m^*)^{3/2}\sqrt{2E}}{\pi^2 \hbar^3} \qquad (4)$$

where m^* is the effective mass of the carrier. For carrier density $n > 4\times10^{19}$ cm^{-3}, the measured S results were quite consistent with the theoretical calculation of S_c values using Eq. (3), as shown in Fig. 2, implying that the influence of an impurity band was negligible.
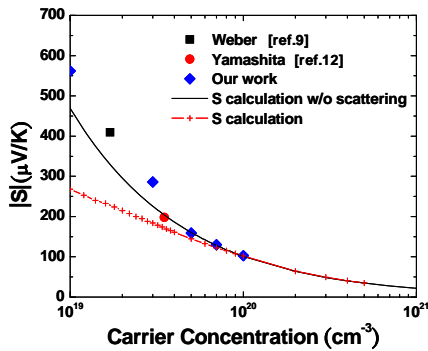

Fig.2 Absolute Seebeck coefficient as a function of carrier concentration.

Simultaneously, the measured σ, as function of n, fits the conductivity calculations based on an empirical relationship between μ and n for bulk silicon, as shown in Fig. 3.[11] The measured σ results suggest that surface scattering in the heavily doped SiNWs had a negligible effect on the electrical conduction.
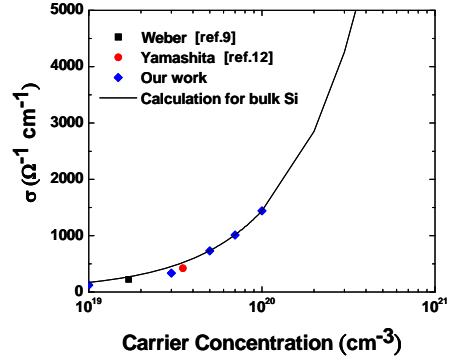

Fig.3 Electrical conductivity as a function of carrier concentration.

For $n < 4\times10^{19}$ cm^{-3}, the marked difference in the S_c calculation between Eq. (2) and Eq. (3) can be explained by the effect of the scattering factor. The increase in the measured S value relative to the calculation of Eq. (3) is shown in Fig. 2. Furthermore, two reported literature values for S are re-plotted in Fig. 2.[9,12] These experimental results regarding S enhancement suggest that the increased S values can be attributed to the contribution of phonon drag component of the S value. The component of phonon drag is due to momentum transfer from the phonon system to the electron system caused by electron-phonon scattering. Simultaneously, the measured dependence of σ on carrier density, n, is lower than the same σ conductivity calculation for bulk silicon. This clearly indicates that, for $n < 4\times10^{19}$ cm^{-3}, the lower σ can be explained by the decrease in μ which is partly due to the electron-phonon scattering. In addition, the contribution of the phonon drags to the total S can be evaluated by the expression $(S - S_c) / S$, where S_c is equivalent to the calculation of Eq. (3). Around 20% of the phonon drag effect contributing to the total S was found to be comparable with the values reported in literature.[9] Especially for $n = 3.5\times10^{19}$ cm^{-3}, the S value appeared to be consistent

with the calculation of S_c using Eq. (3). This implies that the S_{ph} is likely to vanish due to a smaller mean free path of the phonons. Therefore, the carrier concentration of approximately 4×10^{19} cm^{-3} was used for differentiating between the contributions of the phonon and/or carrier components to the S value. Finally, the thermoelectric PF was evaluated by the product of the square of S, shown in Fig. 2, and the σ, shown in Fig. 3, and the corresponding PF results are shown in Fig. 4. To maximize the PF, the optimum carrier concentration was found to be approximately 2×10^{19} cm^{-3}, indicating that the maximized PF is due to S enhancement caused by the effect of phonon drag.
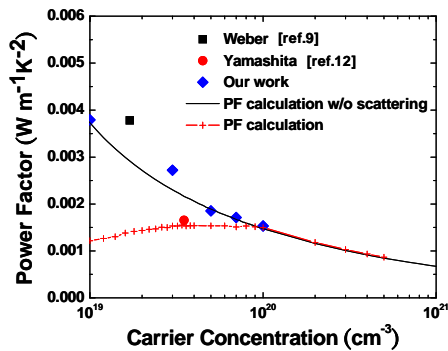

Fig.4 Thermoelectric power factor (PF) as a function of carrier concentration.

IV、Conclusion

The thermoelectric PF for SiNWs with heavily doped carriers having concentrations, ranging from 1×10^{19} cm^{-3} to 1×10^{20} cm^{-3}, was re-examined. When the carrier concentration was greater than 4×10^{19} cm^{-3}, the decrease in S corresponding to the increased concentration agreed with the theoretical calculations of S_c, implying that the influence of an impurity band was negligible. For carrier concentrations less than 4×10^{19} cm^{-3}, an increase in S and a decrease in the electrical conductivity, σ, relative to the values calculated for bulk silicon are observed, further supporting the contribution of phonon drag to the S. The carrier concentration for maximizing the PF was determined to be approximately 2×10^{19} cm^{-3}.

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