Si$_{1-x}$Ge$_x$ nanowire arrays for thermoelectric power generation

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Thermoelectricity offers an excellent clean energy generation opportunity and has attracted renewed attention in the last few decades. The low conversion efficiency and high costs currently limit its practical application. Much effort is still needed to enhance its efficiency and reduce its cost. Nanostructures have been proven to greatly enhance the thermoelectric figure of merit (ZT) because of increased phonon scattering at the interfaces. It has been demonstrated that single Si nanowires (NWs) exhibit a 60 times higher ZT than Si bulk$^1$. Meanwhile, SiGe alloys can also reduce the thermal conductivity via alloy scattering$^2$ without deteriorating the other performance parameters such as Seebeck coefficient, $S$ and electrical conductivity, $\sigma$. SiGe NWs thus promise to offer even better thermoelectric performance than Si. In this work, we will show our recent research results on the fabrication and thermoelectric characterisation of SiGe nanowire arrays (NWAs). The NWAs are arrays of millions of parallel upstanding NWs attached to Si bulk, rather than single NWs as studied before.

SiGe material with Ge content of 20%, 30% and 40% is grown by MOCVD (metal organic chemical vapour deposition). A 3-4 $\mu$m graded buffer layer is grown to overcome the lattice mismatch between Si and SiGe, followed by the growth of a 3 $\mu$m relaxed, constant composition, SiGe layer. The SiGe NWAs are fabricated using metal assisted electroless chemical etching$^3$ (MACE). The length of the NWs is between 10 and 20 $\mu$m attached to 500 $\mu$m bulk Si. The diameter is between 50 and 200 nm. Fig. 1 gives the SEM and EDX of the etched NWAs with two different MACE processes. The MACE process was optimised for Ge retention.

The thermo-electric properties of the NWAs are measured using the setup in Fig. 2a, constructed for thin film characterisation that prevents direct connection of the measurement leads. The measurement error is greatly reduced by using Ag foil to decrease the thermal resistance of the Cu - NWA interface. The pressure applied also reduces thermal and electrical interface resistances. A Seebeck coefficient of $S \approx 1.1$ mV/K is measured for the SiGe NWAs/Si bulk composite and is independent of Ge fraction, consistent with the theoretically expected value. The temperature drop across the SiGe NWA is consistently larger than across a similar Si NWA, indicating reduced thermal conductivity of the SiGe NWs.

A thermo-electric generator (TEG) is constructed using one p-n junction (fig.3a). A constant pressure and uniform heat flux input is applied to each TEG leg. It is found that both the NWA structure and SiGe boosts the output power of the TEG (Fig. 3b-3d). The TEG using Si NWAs shows higher output power than bulk (Fig.3 b). The output power and internal resistance of the SiGe NWA TEGs are better than the Si NWA TEG. The use of SiGe improves the output power with a factor of 8 in the bulk TEG configuration. The use of SiGe NWAs in the p-leg only, increases the output power by a factor of 5 in comparison with the Si NWA TEG. These improvements are due to the reduction of the thermal conductance of the SiGe NWs and the reduction of the electrical contact resistance of the SiGe-based wires while the Seebeck coefficient remains unaffected.

This work demonstrates the benefits of SiGe containing NWAs for low power thermoelectric power generation that could be integrated in Si electronics.

References
Figure 1. (a) SEM cross-section of SiGe sample after 2-step MACE. The arrow indicates horizontal etch of the graded composition layer. (b) SEM cross-section of Si$_{0.8}$Ge$_{0.2}$ NWA after 1-step MACE. (c) EDX spectrum of the Si$_{0.8}$Ge$_{0.2}$ NWA taken at the spots sp4 and sp6 indicated in image (b).

Figure 2. (a) Seebeck coefficient measurement set up. (b) Seebeck coefficient measurement value.

Figure 3. (a) TEG set-up. (b) Output power of Si bulk vs. Si NWAs TEG. (c) Output power of Si bulk vs. SiGe bulk TEG. (d) Output power of Si NWA vs. SiGe NWAs TEG.