GREEN Silicon: ICT FET Project No. 257750
Deliverable D2.2 Report on ZT Measurements

9th November 2011

The objectives of task 2.2 and deliverable 2.2 was to measure the electrical (4-terminal measurements) and thermal transport (3ω technique and thermal AFM) through (a) bulk silicon (reference) (b) Si/SiGe superlattices and (c) Ge quantum dots in a Si or SiGe matrix allowing electrical conductivity, thermal conductivity, ZT and thermoelectric efficiency to be determined.

Devices were designed in a Hall bar configuration and to allow the substrate to be removed so that all the required measurements could potentially be undertaken on a single device (see Fig. 1 and 2). For bulk p-type silicon, a Seebeck coefficient of 150 μV/K, an electrical conductivity of 125000 S/m and a thermal conductivity as measured by the 3ω technique of 143 W/mK providing a ZT of 5.9 x 10^{-3} at 300 K.

For the Ge/SiGe wafers grown there were a number of issues which made the fabrication of devices problematic and also resulted in large uncertainties of the measured thermal conductivities, Seebeck coefficients and ZT values. These problems included exfoliation of the wafers after growth (solved by slow cooling) and high dislocation densities in the thin virtual substrates (up to 10^9 cm^{-2}). A number of approaches are being attempted to reduce the dislocation densities including using low temperature seed layers, Ge island growth followed by anneals then the $Si_{1-y}Ge_y$ strain growth and 2 or multiple step buffers. The major problems were related to measuring the thermal conductivity and the Seebeck coefficient. Due to the residual strain in all of the strain symmetrised superlattices, many of the large Hall bars broke when the silicon substrate was removed (Fig. 3). We are presently making smaller Hall bars where this will be less of an issue. Therefore all measurements have used samples where the substrate has not been removed.

Table 1 shows the measured electrical conductivity for a large range of samples with the highest conductivity being 118,500 ± 15,000 S/m. The large standard deviation is related to the non-uniformity of the material in this sample since it was a wafer with exfoliation and only samples near the edge of the wafer remained intact for measurements. The measured Seebeck coefficient was 150 ± 13 μV/K which is very similar to the bulk Si and suggests that the substrate still has significant contribution to the Seebeck coefficient and must be removed for accurate measurements. The differential 3ω produced thermal conductivity measurements ranging from 0.17 W/mK to 1.27 W/mK, the former value should be more

Wafer_Sample	Design	x %	N_A (cm^{-3})	Material Thickness	σ (S/m)
8482_E4	p-Ge design 2	75	1 x 10^{19}	11.34 μm	3,490 ± 290
8557_J6	p-Ge design 2	75	1 x 10^{19}	3.268 μm	118,500 ± 15,000
8569_I8	p-Ge design 2	75	1 x 10^{19}	6.048 μm	38,660 ± 1,460
8569_I7	p-Ge design 2	75	1 x 10^{18}	6.426 μm	25,850 ± 2,620
8569_F2	p-Ge design 2	75	1 x 10^{19}		41,100 ± 11,600
8579_E2	p-Ge design 1	80	1 x 10^{19}	6.048 μm	72,730 ± 29,700
8572_D2	p-Ge design 2	75	1 x 10^{19}	6.804 μm	26,012 ± 11,000

Table 1: A summary of the Hall bar measurements of electrical conductivity for the different samples.

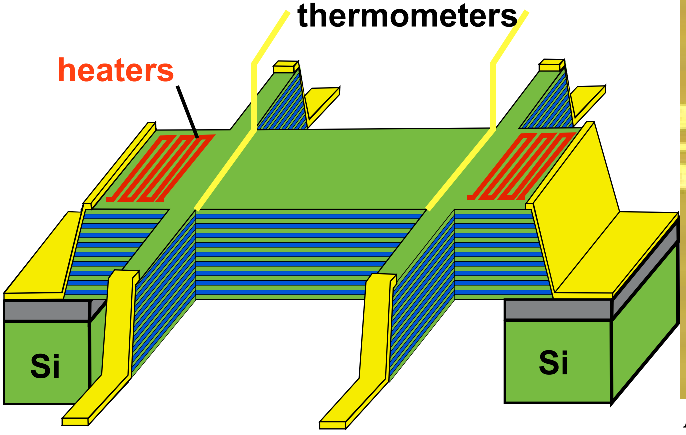

***Fig. 1**: A schematic diagram of the Hall bar device for measuring Seebeck coefficient, electrical conductivity and thermal conductivity.*

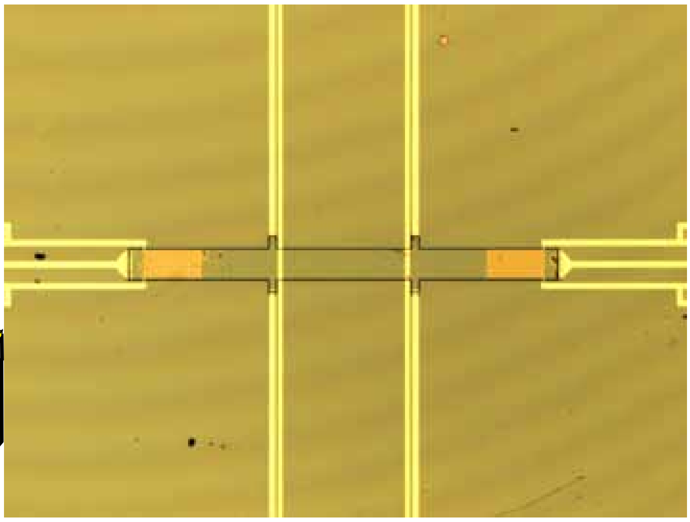

***Fig. 2**: Optical microscope images of the Hall bar samples with Ohmic contacts, heaters, voltage probes and thermometers before the substrate is removed. We now have a high yield up to this point in the process.*

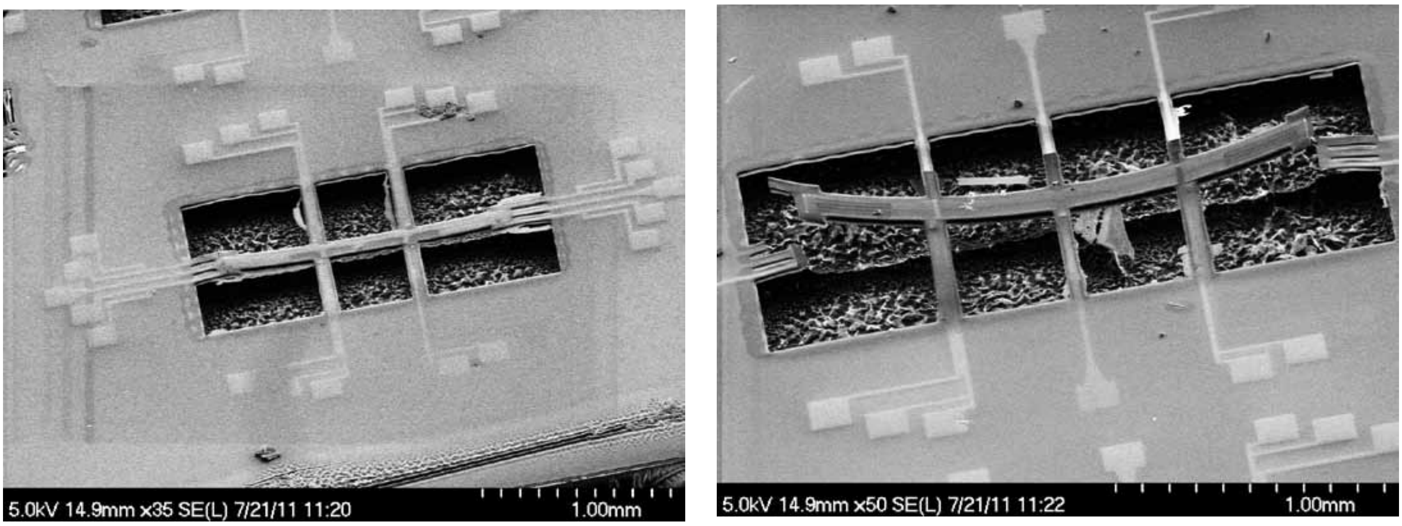

***Fig. 3**: SEM images of Hall bar samples after a surface isotropic etch to remove the Si substrate from underneath the Hall bar. The samples are from wafer 8572. The sample on the right is clearly broken due to the strain in the system. However, not all the heater and thermometer contacts on the left hand side are intact.*

accurate as it is at higher frequency and therefore at a shallower depth in the material. Thermal AFM measurements, however, produce the much larger thermal conductivity values of 6.35 ± 1.02 W/mK. Table 2 shows the maximum and minimum possible values for ZT taken using the maximum and minimum α, σ and κ values ± the standard deviation to demonstrate the complete range of uncertainty. The present measurements suggest almost 2 orders of magnitude for the uncertainty. As the 3ω technique is unlikely to be a valid technique for the present superlattices since it requires a thin uniform layer for measurement, the thermal AFM measurements should be more correct for the thermal conductivity measurements. These suggest a ZT value of 0.126 ± 0.085 W/mK where the uncertainty is calculated using

$$(\frac{\Delta ZT}{ZT})^2 = 2(\frac{\Delta\alpha}{\alpha})^2 + (\frac{\Delta\sigma}{\sigma})^2 + (\frac{\Delta\kappa}{\kappa})^2 + (\frac{\Delta T}{T})^2$$

We are now working with the U.K. standards agency, NPL to help produce more accurate thermal conductivity measurements for thermoelectric material characterisation. It is clear from the research in the first year of the project that the standard 3ω technique is not suitable and the thermal AFM technique must be used for accurate results. Also the substrate must be removed from samples to allow accurate thermal transport for measurements. We are presently making smaller Hall bars where the stress at the ends is less to allow accurate measurements to be completed.

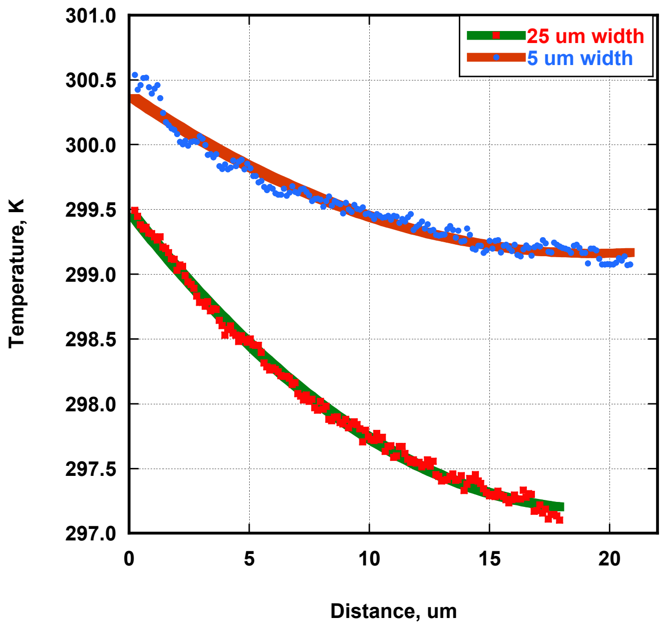

***Fig. 4**: Thermal AFM measurements on sample 8557_J6. The thermal conductivity is measured to be (red dots) 6.36 ± 1.02 W/mK.*

Comment	σ (S/m)	α (μV/K)	κ (W/mK)	Z	T (K)	ZT
Maximum ZT value (mean ± standard deviation)	128500	163	0.17	0.020083	300	6.02
Maximum 3ω κ	118500	150	1.27	0.0020994	300	0.630
Mean values from max / min of κ	116000	150	3.365	0.00077563	300	0.233
Thermal AFM κ with mean σ	118500	150	6.36	0.00041922	300	0.126
Minimum ZT value (mean ± standard deviation)	103500	137	7.37	0.0002636	300	0.0791

Table 2: The maximum and minimum possible ZT values obtained from measurements on sample 8557_J6 - a p-Ge modulation doped quantum well of design 2 with a thin $Si_{0.25}Ge_{0.75}$ strain relaxation buffer.