GREEN Silicon: ICT FET Project No. 257750
Deliverable D2.5 Report on Optimised Material

Update on 25th June 2013

This deliverable is to review the work in Workpackage 2 and determine from the theoretical modelling and the experimental results to date which is the optimum thermoelectric material in the project that can be used for the thermoelectric generator fabrication in the third year of the project.

This is an updated report with additional thermoelectric charcterisation of both lateral and vertical p-type Ge/SiGe designs and n-type vertical Ge/SiGe designs. Due to doping segregation effects, the n-type lateral Ge quantum wells had poor electron conductivity (all the material was doped rather than just the quantum wells).Table 1 presents the best p-type lateral quantum well results at 300 K along with a comparison of other bulk materials. Complete characterisation and analysis is now available in J. Appl. Phys. 113, 233704 (2013). Fig. 1 demonstrates the complete set of characterised lateral p-type Ge quantum well samples. Temperature dependent measurements between 300 K and 500 K on the 8.3 nm Ge quantum well samples (Fig. 2) demonstrates a small increase in ZT with increasing temperature.

Sample	QW / barrier-width (nm)	σ (S m^{-1})	κ (W m^{-1}K^{-1})	α (μV K^{-1})	ZT (300 K)	$\alpha^2\sigma$ (WK^{-2}m^{-1})
p-Sb_2Te_3	bulk	83,300	2	260	0.84	0.00563
p-Si	bulk	11,100	148	148	0.00049	0.00243
p-Ge	bulk	30,300	59.5	300	0.014	0.00273
p-$Si_{0.3}Ge_{0.7}$	bulk	25,000	6.3	90	0.013	0.00126
p-Ge/$Si_{0.25}Ge_{0.75}$	9.1 / 17.1	77,200	19.9±4.7	280 ± 1.1	0.091 ± 0.022	0.00603 ± 0.00005
p-Ge/$Si_{0.25}Ge_{0.75}$	6.5 / 10.0	27,900	4.0 ± 2.1	255 ± 3.8	0.135 ± 0.074	0.00182 ± 0.00006

Table 1: Laterial p-type modulation doped Ge quantum well material results and comparison with the literature.

Table 2 presents the p-type vertical results at 300 K. The ZTs are not quite as good as the best lateral values but they are only 33% lower. The results from Fig.1 and Table 2 suggest that lowering the Ge content in the barriers should result in reduced interface roughness scattering and therefore higher ZT. New sample designs

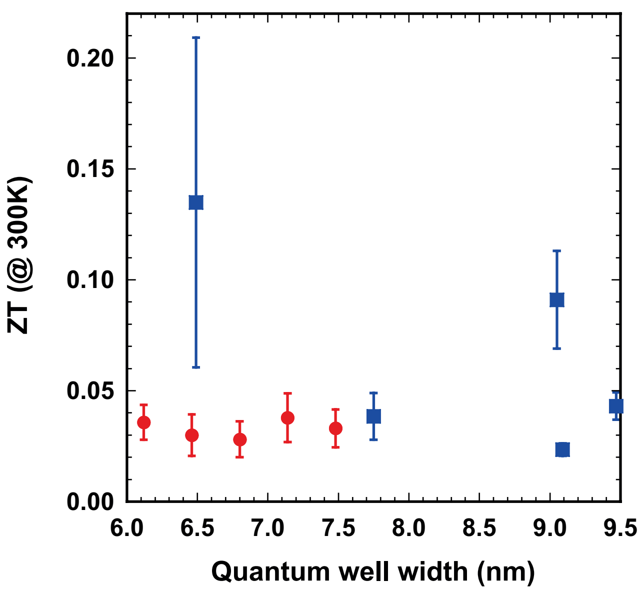

Fig. 1: The ZT for modulation doped p-Ge quantum wells as a function of quantum well width.

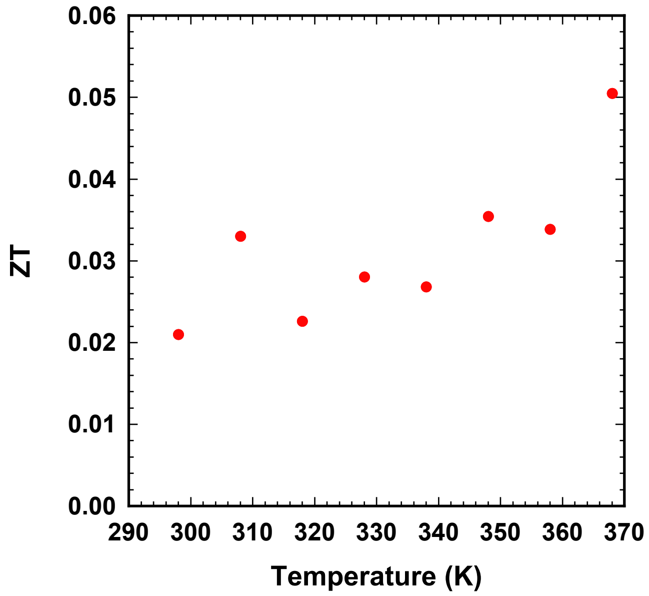

Fig. 2: The ZT for modulation doped 8.3 nm p-Ge quantum wells as a function of temperature.

have been produced and new wafer growths are planned to test this hypothesis.

Sample	QW /barrier-width (nm)	σ (S m⁻¹)	κ (W m⁻¹K⁻¹)	α (μV K⁻¹)	ZT (300 K)	α²σ (WK⁻²m⁻¹)
p-Sb_2Te_3	bulk	83,300	2	260	0.84	0.00563
p-Si		11,100	148	148	0.00049	0.00243
p-Ge		30,300	300	59.5	0.014	0.00273
p-$Si_{0.3}Ge_{0.7}$		25,00	6.3	90	0.013	0.00126
8950	2.85	8,633	5.06±0.43	299	0.081	0.0013
8957	2.85	14,099	5.55±0.25	113	0.09	0.00017
8961	1.1	13,805	5.07±0.03	91.8	0.007	0.00012

Table 2: Vertical p-type Ge/$Si_{0.5}Ge_{0.5}$ superlattice designs and comparison with bulk values.

Table 3 presents the results for the n-type vertical designs at 300 K. The best ZT of 0.4 is within a factor of 2 of the best Bi_2Te_3 at room temperature but with a power factor which is 3 times larger than Bi_2Te_3. This is the highest recorded ZT from a non-Te containing material at room temperature. Companies want to remove Te as it is the 9th rarest element on earth and non-sustainable. Initial temperature dependent measurements of the Seebeck and thermal conductivity are in Fig. 3 suggesting higher ZT values at higher temperature as expected from theory. The electrical conductivity measurements are in progress.

Sample	QW /barrier-width (nm)	σ (S m⁻¹)	κ (W m⁻¹K⁻¹)	α (μV K⁻¹)	ZT (300 K)	α²σ (WK⁻²m⁻¹)
n-Bi_2Te_3	bulk	120,000	1.2	–160	0.768	0.00372
n-Si	bulk	16,700	148	–95	0.00031	0.00015
n-Ge	bulk	123,000	59.9	–308	0.032	0.0117
n-$Si_{0.15}Ge_{0.85}$	bulk	26,300	6.7	–367	0.159	0.0354
8719	3.0 / 1.5	49,800	7.75	–455	0.40	0.0103
8717	10.0 / 1.9	55,900	8.63	–320	0.20	0.0057
8802	10.6 / 2, 3	74,100	7.30	–295	0.26	0.0065
8722	9.5 / 2, 3, 4	51,600	6.57	–403	0.38	0.0084

Table 3: Vertical n-type Ge/$Si_{0.2}Ge_{0.8}$ superlattice designs and comparison with bulk values.

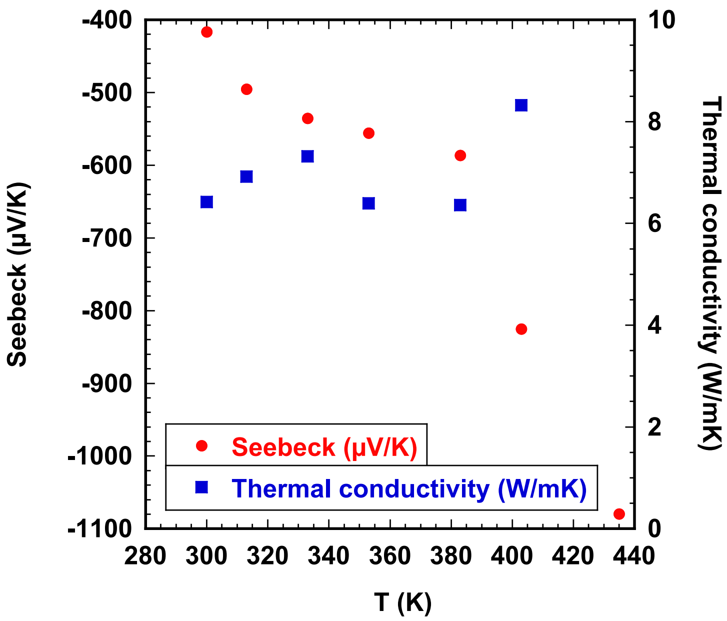

Fig. 3: The Seebeck and thermal conductivity for 8719 vertical 3 nm Ge QW superlattice versus temperature.

The results in table 3 and Fig. 3 demonstrate significantly higher performance from the vertical n-type designs and suggests the decision to proceed with vertical module designs was the correct one. These are significantly easier to fabricate than the lateral module designs but also the vertical material overall has higher performance as described above in this deliverable.