GREEN Silicon: ICT FET Project No. 257750
Deliverable D2.4 Delivery of Quantum Dots Inside a Matrix Material

10th September 2011

The objective of task 2.3 was to produce Ge quantum dots inside a Si or $Si_{1-x}Ge_x$ (x << 1) matrix for thermoelectric material. The bandstructure of Ge/Si is such that Ge forms a conduction band barrier to electrons when grown directly on Si or low Ge content $Si_{1-x}Ge_x$ (i.e. x << 1) but it forms a quantum well to holes. Therefore our initial experiments are investigating n-type quantum dot structures that have the potential to scatter the phonons thereby reducing the thermal conductivity. The quantum dots will also scatter the electrons but the aim is to find a dot size, density and spacing that will scatter phonons more than the electrons.

The first calibration samples to be grown were all single Ge layer samples with different growth temperatures and Ge thicknesses to determine through physical characterisation (AFM, TEM and XRD) the quantum dot height, size, density and distribution as a function of growth parameters. Once an optimum was found, two wafers of 50 periods of quantum dots were grown vertically with n-type doping and these will be fabricated into devices to allow electrical and thermal measurements. The list of samples grown and delivered is given in Table I.

Wafer ID	Date Grown	Growth T	Ge thickness	Notes	XRD Ge content
56610	09/03/2011	600 ˚C	1 nm	Single layer calibration sample	96.3±0.5%
56611	11/03/2011	500 ˚C	1 nm	Single layer calibration sample	83±1%
56612	23/3/2011	400 ˚C	10 nm	Single layer calibration sample	
56618	28/3/2011	400 ˚C	1 nm	Single layer calibration sample	63±1%
56621	4/4/2011	400 ˚C	0.5 nm	Single layer calibration sample	
56635	19/4/2011	350 ˚C	0.5 nm	Single layer calibration sample	
56640	27/4/2011	375 ˚C	0.5 nm	Single layer calibration sample	
56696	25/7/2011	400 ˚C	50 x 1 nm	Dot multilayer n-type	
56700	27/7/2011	500 ˚C	50 x 1 nm	Dot multilayer n-type	

Table I: The full list of 9 delivered Ge quantum dot wafers. The first samples were calibration samples aimed at understanding the quantum dot density and size before 2 multilayer samples were grown for thermoelectric characterisation.

TEM investigations of the first Ge-dot samples (56610 - typical dot size around 25 nm) determined the height of the dots to be 6-8 nm. If the native oxide is included than the dot height is 9±2 nm. This is the same

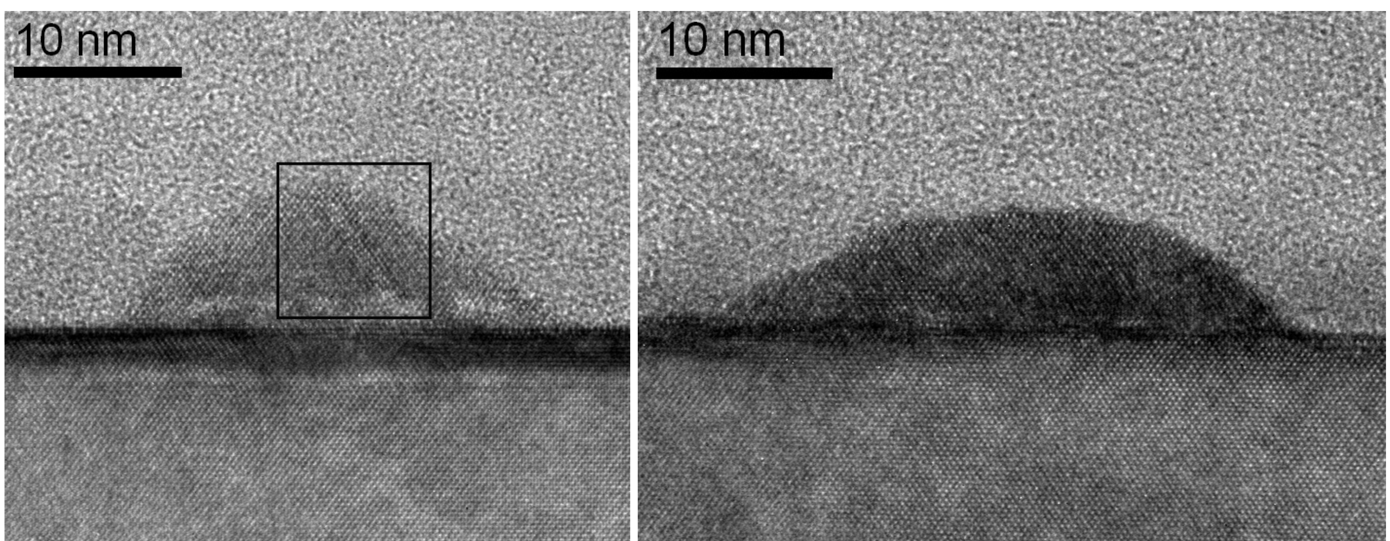

Fig. 1: TEM images of the single quantum dot calibration sample 56610. The left hand image indicates a stacking fault in the quantum dot.

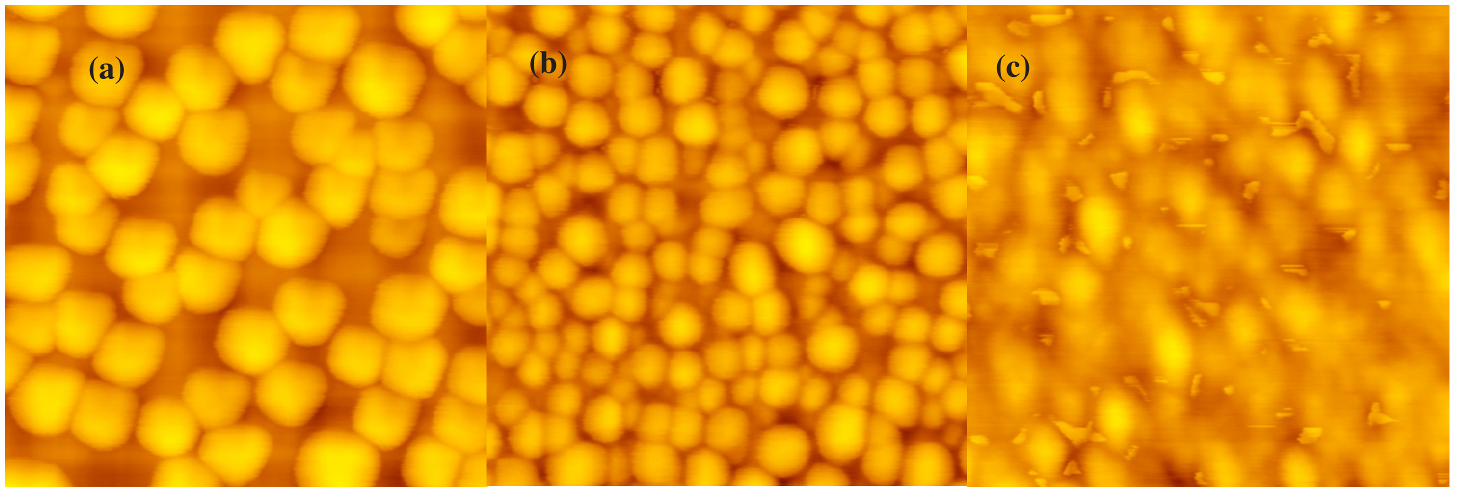

Fig. 2: AFM measurements over a 5 x 5 μm area for wafers (a) 56610 (z-range 15.4 nm)(b) 56611 (z-range 11.1 nm) and (c) 56621 (z-range 5.4 nm).

height as deduced from XRD-measurements, hence demonstrating good correlation between the TEM and XRD measurements. With respect to structural details the TEM investigations revealed the presence of stacking faults within many dots (Fig. 1). Further investigations will have to show if and how this can be avoided.

Fig. 2 shows AFM measurements for the samples with reducing growth temperature. The dot height is reduced as the growth temperature is reduced but so is the Ge composition of the dot. While the existence of the islands can be seen from AFM, XRD measurements provide information on the chemical composition from the intensity distribution in reciprocal space. From the peak positions, the lattice parameters and hence the Ge content can be evaluated. This was only possible for the samples with the largest quantum dot (65510-56618), for all subsequent samples the intensity of the Ge signal was too low. The results are in table I, demonstrating an increasing Si content in the dots as the growth temperature is reduced.

We found another feature, namely a significant minimum of the intensity distribution at the center of the peak (Fig. 3(a)). This, as it turned out from small-angle x-ray scattering experiments, is caused by the positional correlation of the islands: Their minimum distance (center to center) cannot be smaller than their diameter. Since the dots are rather dense, this gives rise to a prominent dip in the distribution function, which is overlaid to the size-dependent structure factor in reciprocal space. From the distance and contrast of this position correlation function measured in small-angle scattering (see Fig. 3), we have evaluated the correlation properties of the SiGe island ensemble. Due to the weak scattering signal this was only able for the sample with the largest dots 56610. For this sample the best fit gives a mean radius of 8 nm with σ size 5 nm, a mean distance of 14 nm with a σ of 14 nm as well. This means that there is virtually no correlation except the minimum distance, i.e., the distribution is only confined by the geometric constraints.

Finally Fig. 3(b) shows an XRD rsm scan along (224) for sample 56700 with 50 periods of Ge quantum dots. The XRD demonstrates good coherence of the lattice constant to the substrate.

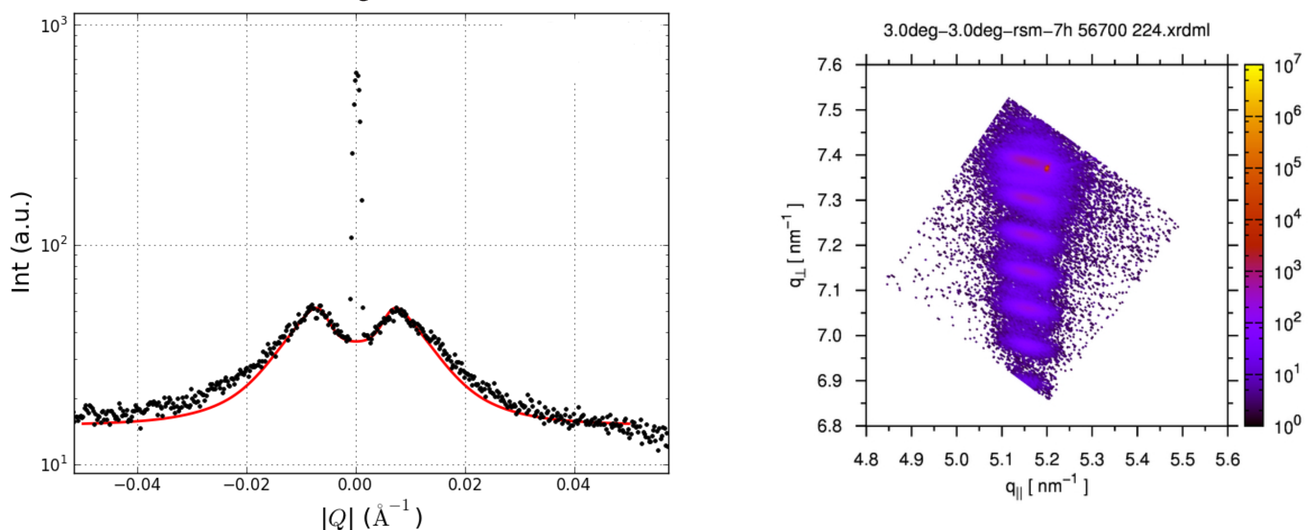

Fig. 3: (a) XRD measurements showing the small angle scattering from sample 56610 and (b) the rsm scan along (224) for sample 56700.