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1.5 μm luminescence of silicon nanowires fabricated by thermal evaporation of SiO

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Silicon nanowires (NWs) fabricated by thermal evaporation of SiO were studied by cathodoluminescence. A band around 1550 nm (0.8 eV) was observed. It appears above 225 K and its intensity increases with increasing temperature. The broad band consists of the defect-related D1 and D2 lines and is supposed to be formed by extended defects within the NWs that are decorated with oxygen. Moreover, luminescence bands are found that are related to Si oxide and/or the interface between Si and Si oxide. In addition, the Si band-to-band line and the G center are observed.

Optical interconnection is needed for future integrated circuits. Many key photonic components compatible with CMOS technology have already been demonstrated, as for example a fast Si based electro-optical modulator, allowing the use of continuous-wave light sources. However, a silicon based light emitter which can be integrated in the chip is still lacking. The desired light emitter should exhibit a high luminescence efficiency at room temperature (RT) and emit at about 1.55 μm or 1.3 μm [1, 2].

Semiconductor nanowires exhibit new properties. Recently, it was shown that the light extraction from an InGaN/GaN LED was markedly enhanced by using nanorod/nanowire arrays instead of the entire area of the LED [3]. This approach could also be used for silicon if Si nanowires (Si-NWs) with appropriate luminescence behaviour are available. Si is believed to develop a direct band gap in nanometer-sized structures. Calculations showed that [110] oriented Si-NWs have a direct bandgap. However, the density of states was found to be very small at the conduction band edge [4]. Er surface-enriched Si-NWs were reported to cause the desired light emission at about 1.55 μm [5]. Here we show that Si-NWs are capable to yield efficient RT emission around 1.55 μm without an additional Er doping.

Si-NWs were fabricated on top of p-type (111) Si substrate with 0.001 Ω cm resistivity by thermal evaporation of Si monoxide [6, 7]. Transmission electron microscopy (TEM) reveals that the NWs have a diameter of about 20–30 nm, a length of tens of micrometers and exhibit a crystalline structure. Oxygen was detected at the NWs by energy-dispersive X-ray spectroscopy (EDX) because the Si core of the NWs is surrounded with a Si oxide shell.

The NWs were investigated by cathodoluminescence (CL) using a Zeiss EVO 40 scanning electron microscope equipped with a cold stage, a Gatan MonoCL system and a Hamamatsu detector. The measurements were executed with an acceleration voltage of 7 kV and a beam current of about 50 nA. The temperature of the sample was varied between 78 K and RT. The sample was scanned usually over an area of about thousand μm^2 with normal incidence of the electron beam to the wafer surface.

Figure 1 shows a characteristic spectrum of the Si-NWs measured at 78 K. Three main bands can be clearly seen. The bands 1, 2 and 3 appear at about 660 nm, 920 nm and 1280 nm, respectively. Upon increasing temperature their intensities are found to decrease but a new band around 1550 nm appears, see Fig. 2. Details about the

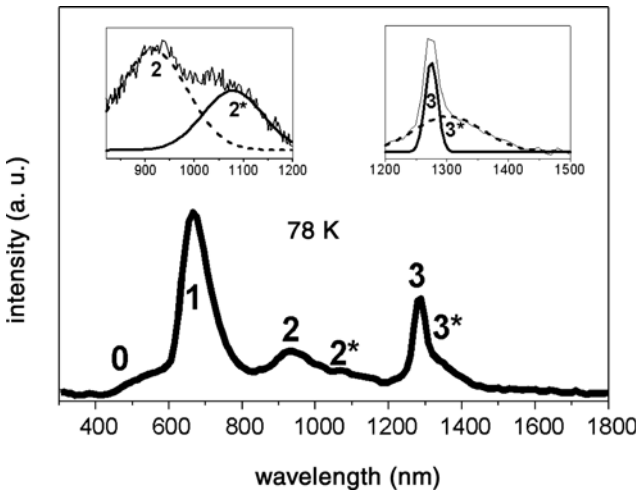

Figure 1 CL spectrum of Si nanowires measured at 78 K. The bands 1, 2 and 3 can clearly be seen. Additional lines 0, 2* and 3* can be found by deconvolution; for lines 2* and 3* compare insets.

spectra, which will be discussed below, are summarized in Table 1.

The spectral region around band 2 exhibits two features, namely peak 2 at 920 nm and an additional peak 2* at 1080 nm, see left inset in Fig. 1. Detailed analysis of the spectral region around band 3 is represented in the right inset of Fig. 1. It shows a sharp peak 3 at 1280 nm and a broad peak 3* with a maximum at about 1320 nm. On the left shoulder of peak 1 a band in the range 450–550 nm, denoted here band 0, was found by deconvolution. Due to decreasing sensitivity of the CL system on the low wavelength side the measured intensity for band 0 is strongly reduced. We believe that its real position is closer to 450 nm than to 550 nm.

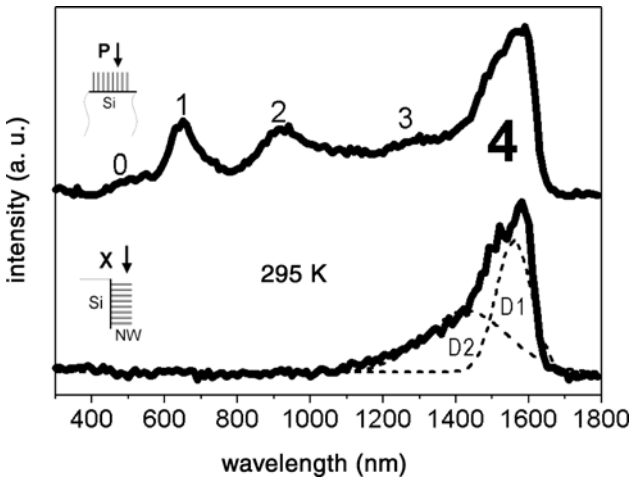

Figure 2 CL spectra of Si nanowires measured at room temperature exhibiting a new intensive band 4 around 1550 nm. The upper spectrum (P) was observed with planar incidence of the electron beam and the lower spectrum (X) was measured on the cross-section after cleaving the sample.

Table 1 Features deduced from the luminescence spectra.

peak/band	wavelength (nm)	cause
0	~460	Si oxide and
1	660	interface Si/Si oxide
2	920	2nd order of peak 0 (?)
2*	1080	BB line of Si
3	1280	G center
3*	1320	2nd order of peak 1
4	1550	D1 line
	1420	D2 line

Peaks 0, 1, 2 and 3* are related to Si oxide and/or the interface between Si and Si oxide. Recent observation of the peaks 0, 1 and 2 in CL spectra, emitted from multiple quantum wells of alternating Si and SiO_2 layers on quartz substrate, confirms this view [8].

Features related to band 0 were reported in the literature. A dominating band at 460 nm, arising from the interface between the SiO_2 layer and Si substrate, was observed by CL [9]. A similar band was reported for Si-NWs fabricated by evaporation of SiO [10]. It was attributed to the oxygen vacancy in Si oxide. Peak 2 (920 nm) might be interpreted as 2nd order of peak 0 (460 nm). However, the fact that the intensity of peak 0 is much smaller than that of peak 2 is in opposition to this view.

Features related to peak 1 are reported by photoluminescence (PL) analysis of Si-NWs surrounded with a Si oxide shell [10, 11]. They are attributed to Si oxide and the Si/Si oxide interface. Peak 3* at about 1320 nm is the 2nd order of peak 1 (660 nm).

Peak 2* at 1080 nm reflects clearly the band-to-band (BB) transition in crystalline Si, see e.g. [12]. It can be generated by radiative recombination within the Si-NWs and/or in the Si substrate, but Auger recombination is believed to suppress its formation in the highly doped substrate. The sharp peak 3 at 1280 nm (0.97 eV) can be ascribed to the G center. The G center was observed by CL to be connected with grain boundaries/twins in Si [13]. Consequently, its appearance indicates the existence of twin boundaries within the Si-NWs. Indeed, twins and other extended defects have been directly observed by TEM within Si-NWs, e.g. [14–16].

The G center is known to exist in carbon-rich Si, i.e. its appearance points to carbon (C) contamination of the NWs. A C-induced twinning process has been reported for Si as a rather general process where a single layer of C atoms is incorporated in the twin planes [17]. For example, twin boundaries in EFG and block-cast Si were found to accommodate C atoms, e.g. [17]. We suppose that also twins in the Si-NWs accommodate a large portion of C. Thus, we believe that according to the above discussions the formation of peaks 0, 1, 2, 2* and 3* is not related to C, except for the G center (peak 3).

Figure 2 shows CL spectra measured at RT with planar geometry (P) and, after cleaving the sample, with the beam

scanning the cross-section in the region of the NWs (X). The bands that are found for low temperature (see e.g. Fig. 1) exhibit at RT a smaller intensity or disappear. However, an intensive new band 4 is observed around 1550 nm (about 0.8 eV). In spectrum X only this band can be seen. Band 4 becomes visible at about 225 K and its intensity increases with increasing temperature. A similar band around 0.8 eV (1550 nm) was reported for nanocrystalline Si, namely for CVD-grown nanocrystalline Si films [18] and for Si nanocrystals fabricated by mechanical milling of Si [19]. Within the nanocrystals a high density of extended defects was found by TEM in both types of samples.

In general, dislocations/extended defects in Si are known to form the quartet of the D1–D4 lines in the luminescence spectrum, see e.g. [20]. As shown in Fig. 2, the broad band 4 consists of two lines. The dashed lines, plotted in spectrum X, display a strong peak at about 1550 nm and a broad peak with a maximum at about 1420 nm that can be ascribed to the D1 and the D2 line, respectively. Recently, we have reported that for specific dislocation networks in Si the D1 line dominates the whole spectrum, see e.g. [2]. We also found that oxygen accommodated at the dislocation network enhances the intensity of this D1 emission [1].

Accordingly, the broad band 4 emitted from the Si-NWs fabricated by evaporation of SiO is supposed to be caused by extended defects within the NWs that are contaminated with oxygen. We also assume that the interface between the Si oxide shell and the Si core of the NWs acts as passivation suppressing non-radiative recombination. The observed strong RT emission around 1550 nm of the Si-NWs, that appears without additional Er doping, exhibits a promising feature for application.

We can exclude that the electron bombardment, used here for CL analysis, creates defects that emit the band-4 luminescence. PL measurements with an excitation wavelength of 514 nm showed a broad luminescence band with a maximum between 1500 and 1700 nm [21], which is similar to band 4 found by CL. Furthermore, after deconvolution of the PL spectrum the D lines (even D4 and D3) were extracted, pointing to the existence of crystal defects in the NWs. Such crystal defects cannot be formed by a 7 keV electron bombardment, used here for CL.

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