DISLOCATION-INDUCED DEFECT LEVELS IN SILICON

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Abstract

High purity samples containing dislocations were obtained by laser melting and re-crystallization of n-type FZ-Si wafers. The dislocation network were characterized by transmission electron microscopy (TEM) and the influence of copper and hydrogen on the dislocation induced electronic levels was studied by photoluminescence and deep-level transient spectroscopy (DLTS). A correlation between the D-band photoluminescence and DLTS levels could not be established in n-type Si.

Introduction

Extended defects such as dislocations are known to introduce deep electronic states into the band gap of semiconductors. Despite a large number of studies using deep level transient spectroscopy (DLTS) [1]-[7], photoluminescence (PL) [8], [9], [10] and ESR [11] the defect levels of dislocations in silicon are still discussed controversially. Different models developed for the origin of these levels can be classified as follows

1.) "dangling bonds" at the dislocation core which form a one dimensional chain

2.) Isolated point defects in the strain field of a dislocation

3.) Impurity related defects near or at the dislocation core

In order to distinguish between isolated point defects, impurity- and dislocation-related defects we developped a different sample preparation method compared with earlier studies and used a combination of DLTS, PL and transmission electron microscopy (TEM) to characterize the samples.

Of particular interest to us is the relationship between the states associated with dislocations and the presence of Cu.

Experimental

As starting material, we used samples of P-doped Float Zone (FZ) Si wafers ($[P]=5\cdot10^{15}\mathrm{cm}^{-3}$). The wafer surface was melted locally with an Ar^+ laser beam. The melted zone was scanned across the wafer with a speed of 10 cm/s and in the recrystallized traces of the beam (separation 40 μm) dislocations were created with a density n_d between $5\cdot10^7 - 5\cdot10^8\ \mathrm{cm}^{-2}$. During this process the wafer was either heated to 500°C or kept at room temperature. Preparation without heating leads to more residual strain in the samples.

A gas phase extraction procedure where the sample was heated for 6 h at 800°C under a gas flow of HCl gas was applied to remove residual transition metal (TM) impurities. Copper doping was performed by diffusing Cu scratched on the back side of the samples for 10 min at 800°C. Subsequent, rapid quenching prevented Cu precipitation.

Hydrogenation was carried out in the downstream region of a rf-driven hydrogen plasma for 12h at 350°C. Damage of the sample surface by the plasma was prevented by placing a wafer on top of the samples. More details about the sample preparation are given in [12] and [13].

Figure 1: TEM image of straight 90° dislocations.

After polishing the samples mechanically which removes a layer of 1 - 3 μm thickness and smoothens the corrugated surface gold Schottky contacts were evaporated. For the DLTS-measurement a standard lock-in set up based on a BOONTON 7200 capacitance bridge was used while the PL-measurements were performed with an Ar$^+$-Ion laser with λ = 514.5 nm and P_a = 150 mW at 4.2 K.

The structure of the dislocation network has been investigated with TEM and HREM using JEOL 4000FX, 4000EX and AEI High-Voltage microscopes.

Our samples exhibit straight dislocations ($l \geq 10$ μm) without kinks (see Fig. 1). We observed predominantly two types:

a) 60° dislocations that are dissociated into Shockley partials with a splitting width d_e between 5 and 12 nm (equilibrium width d_e = 5.8 nm).

b) 90° dislocations of the Lomer-Cottrell type with a splitting width of about 8 nm. The region where dislocations were created extends to a maximum depth of approximatly 5μm.
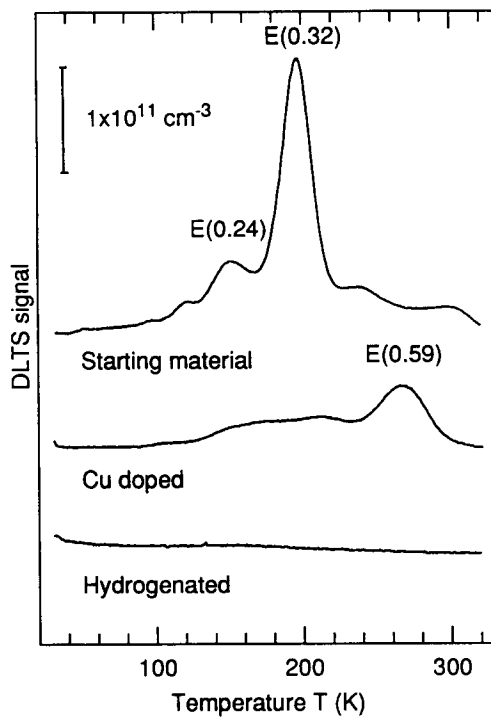
Effect of Cu Doping
a)DLTS

A typical DLTS spectrum of the undoped samples (Fig. 2) shows one dominant peak at 192 K with $E = E_c$-0.32 eV and several minor peaks as listed in table 1.

Peak No.	1	2	3	4	5
T_m [K]	115	149	192	235	266
E [eV]	0.20	0.24	0.32	0.47	0.59

Table 1: Activation energies and positions of the observed DLTS peaks at emission rate $e = 100$ s^{-1}.

The dependence of the capture rate on the filling pulse width was studied and we found, that above 1 ms the pulses were saturated. We therefore chose this pulse width for all our measurements. In our samples we detect concentrations of about $2 \cdot 10^{11}$cm^{-3} which is two orders of magnitude smaller compared to earlier studies on plastically deformed samples (e.g. [1], [6], [7]). The dislocation density, however, is in the same range as for our samples.

After Cu doping, the DLTS spectra changes drastically (Fig. 2): A new peak at 267 K ($E = E_c$-0.59 eV) emerges and the peak at 149 K ($E = E_c$-0.24 eV) remains strong. The formerly dominant peak E(0.32) is very much reduced in height and is comparable with peak E(0.24). Depth profiling experiments showed, that peak E(0.24) has a very pronounced depth dependency and is strong only near the sample surface ($d \leq 1$ μm).

Figure 2: DLTS spectra of a n-type Si sample containing dislocations ($n_d = 5 \cdot 10^7$ cm^{-2}). Emission rate $e = 100$ s^{-1}, filling pulse width $\Delta t=1$ ms; top: Starting material, center: after Cu doping, bottom: after hydrogenation in a hydrogen plasma for 12h at 350°C.

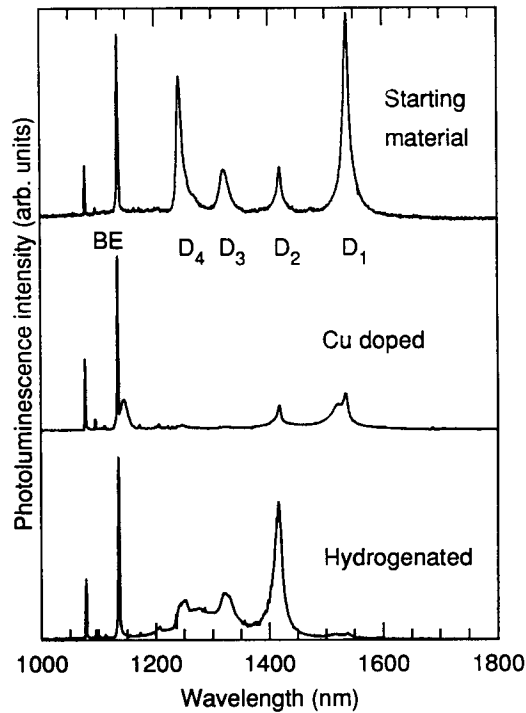Figure 3: Photoluminescence spectra of a n-type Si sample containing dislocations ($n_d = 5 \cdot 10^7$ cm^{-2}) measured with an Ar$^+$ laser ($\lambda = 514.5$ nm) at 4.2 K; top: Starting material, center: after Cu doping, bottom: after hydrogenation (12h at 350°C); BE=band edge luminescence.

b) Photoluminescence

The photoluminescence spectra of the undoped sample (Fig. 3) show the characteristic D-band luminescence of the lines D_1 - D_4 known to appear only when dislocations are present.

After Cu doping the intensity of the luminescence lines D_1 and D_2 is reduced and the intensity of D_3 and D_4 becomes very small (the luminescence signal has been normalized to the band edge luminescence (BE)) (Fig. 3). This result is in agreement with our earlier study [9] which demonstrated that a complete passivation of the D-band luminescence is achieved at higher Cu concentration. The shoulder visible at the D_1 line presumably arises from Cu precipitates at the dislocation.

c) TEM

The location of the Cu-atoms was probed by energy dispersive X-ray (EDX) analysis. This revealed that most of the Cu atoms are trapped at the dislocations, but there is also a smaller fraction in bulk-precipitates. From a weak-beam TEM-image it can be seen that the dislocations are no longer straight. They have moved leaving behind a stacking-fault ribbon and the dislocation line is curved spirally (Fig. 4).

Effect of Hydrogenation

a) DLTS

As a result of hydrogenation, all DLTS peaks vanish (Fig. 2).

b) Photoluminescence

The luminescence spectra measured on the same sample, however, show strong D_2 and D_3 band luminescence (Fig. 3). There is also an additional broad peak at $E \approx 972$ meV ($\lambda \approx 1.275$ μm) that can also be passivated for very long passivation times [13]. The D_1 band vanishes completely and the D_4 band decreases significantly.

Figure 4: Weak beam image taken from defects visible after Cu doping. A spirally curved dislocation is marked by an arrow.

Discussion

The passivation of both the DLTS peak E(0.32) and the D-band luminescence (especially D_3 and D_4) as a result of the Cu doping suggests that these belong to the same energy level which is directly induced by the dislocation. The peaks E(0.59) and E(0.24) seem to be correlated with the Cu-content. This is corroborated by earlier measurements by Prescha et al. [14] who observed after Cu doping a level E(0.54) as strongest DLTS-peak in dislocation-free n-type FZ-Si and we know from our TEM study that there exist in our samples Cu precipitates that are not trapped at the dislocations.

These findings are in disagreement with previous DLTS studies on plastically deformed samples (e.g. [6]) where two main peaks, the so-called D-level (E_c-0.55 eV) and B-level (E_c-0.28 eV) could be observed which are broadened. Probably these peaks are due to impurity centers at the dislocation but a comparison with our results is difficult because the defect concentration in our samples is two orders of magnitude lower than in those used by the authors of [1]-[7] for comparable dislocation densities and the dislocation geometry is different. The internal strain should be higher in the case of plastic deformation and this could be the reason, why the broadening of peaks in our experiment is less pronounced ($\Delta E = 7$meV for E(0.32)).

The fact that hydrogenation completely passivates the levels observed in DLTS but does not passivate the D-band luminescence indicates that a correlation between the defect levels measured in DLTS and in photoluminescence does not exist.

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