Investigation of the recombination activity of misfit dislocations in Si/SiGe epilayers by cathodoluminescence imaging and the electron beam induced current technique

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Misfit dislocations in as-grown and Ni-contaminated Si/SiGe epilayers have been characterized by cathodoluminescence (CL) spectroscopy, cathodoluminescence imaging, and the electron beam induced current technique (EBIC). Dislocations in the as-grown layers had no radiative recombination (*D* bands) and no detectable room temperature EBIC contrast. Following Ni contamination the *D* bands were observed and the EBIC contrast increased. CL dark line contrast is observed by monochromatic imaging of the Si substrate luminescence. The CL dark line contrast was observed from all the dislocations, whether contaminated or as grown. The CL dark line contrast and EBIC contrast show a 1:1 correspondence of the nonradiative recombination at the misfit dislocation and also a semiquantitative agreement with the variation in measured contrast of the individual dislocations.

Photoluminescence (PL) spectroscopy studies have long established that the *D* bands (*D*1–*D*4) are associated with the presence of dislocations in both Si and SiGe alloys.[1,2] The *D*1 and *D*2 bands have been variously attributed to electronic transitions at the stacking fault between the dislocations, transitions at dislocation kinks, or point defects trapped in the strain fields around dislocations, while *D*3 and *D*4 are considered to be associated with electronic transitions at the dislocation core. From most of these investigations there was no clear evidence that impurities played a role in dislocation-related luminescence. However it has been recently demonstrated[3] that dislocation related luminescence could not be observed in the absence of transition metal contamination.

For a more detailed understanding about the origins of the *D*-band luminescence a high resolution scanning technique is required, to gain an insight into the spatial location of the different features. Cathodoluminescence (CL) imaging and spectroscopy have been successfully developed for mapping dislocation structures in both Si and SiGe alloys.[4] Monochromatic imaging of the dislocations showed that *D*3 and *D*4 bands originate on or near the dislocation cores whereas the location of *D*1 and *D*2 seem to originate between the dislocation.

The electron beam induced conductivity (EBIC) technique has been routinely used to study the recombination activity of individual dislocations. EBIC contrast has been found to be extremely sensitive to impurity decoration.[5,6] It has been generally assumed until recently that defects showing no room temperature contrast were assumed to be "clean." However, it has been found that the EBIC contrast may vary significantly with sample temperature. It is now clear that EBIC investigations as a function of both temperature and beam current (I_b) are required for a more detailed understanding of the defect properties.

In this letter we report the first combined EBIC and CL investigation of both as-grown and Ni-contaminated dislocations in Si/SiGe structures. On comparison with EBIC measurements we show a 1:1 correspondence of the nonradiative recombination activity at the misfit dislocations.

This work has used a wide range of Si/SiGe layers grown by chemical vapor deposition using $SiHCl_3$ and GeH_4 at 1120 °C, and supplied by North Carolina State University. The samples consisted of a common structure: A Si capping layer (thickness$=3\ \mu$m) grown on top of a $Si_{1-x}Ge_x$ alloy layer (thickness$=2\ \mu$m) on a Si buffer layer (thickness$=2\ \mu$m) on top of a heavily doped Si(100) substrate. The samples were either untreated or deliberately transition metal contaminated. The Ni-contaminated sample was produced by Ni evaporation on the back face of the substrate followed by rapid transient annealing at 1000 °C for 30 s.

CL measurements were made at $T \approx 5$ K using a JEOL JSM 35C scanning electron microscope (SEM) fitted with an adjustable cold stage, a retractable off-axis paraboloidal collector mirror, and a grating monochromator (Mono CL, Oxford Instruments). The detector employed was a North Coast germanium diode detector. The measurements were carried out with a beam energy of 25 keV and a beam current between 0.1 and 100 nA.

EBIC investigations were performed in a Cambridge Stereoscan S 360 SEM using a Matelect ISM 5 EBIC amplifier fitted with a Kontron image processing system. The EBIC signal was collected using electron transparent Schottky barriers, at a beam energy of 30 keV and a beam current below 0.1 nA.

CL spectra were recorded from a series of uncontaminated samples. All these samples contained misfit dislocations. They all showed the bound exciton features from the heavily doped Si substrate and the majority of these samples showed *D*-band luminescence. However three samples had no observable *D*-band luminescence. Following our original interpretation this would suggest there were no

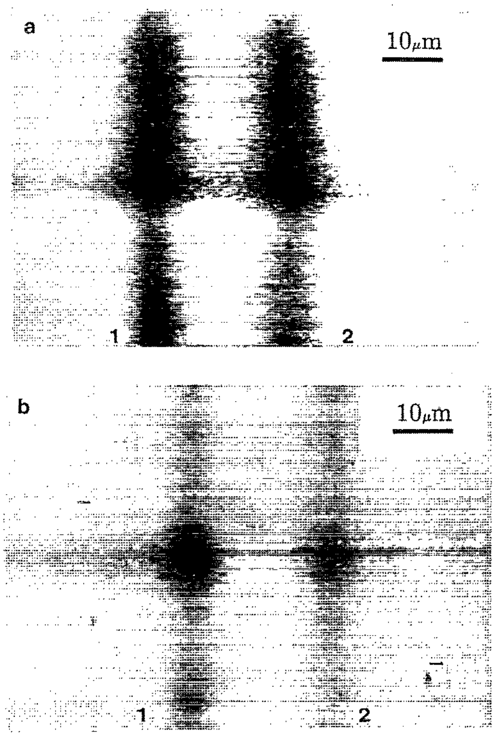

FIG. 1. 1:1 correlation of EBIC and CL imaging of misfit dislocations in the as-grown sample, (a) CL monochromatic image, $E_0=25$ keV, $T=5$ K, $I_b \approx 1$ nA, (b) EBIC image $E_0=30$ keV, $T=80$ K, $I_b \approx 0.1$ nA.

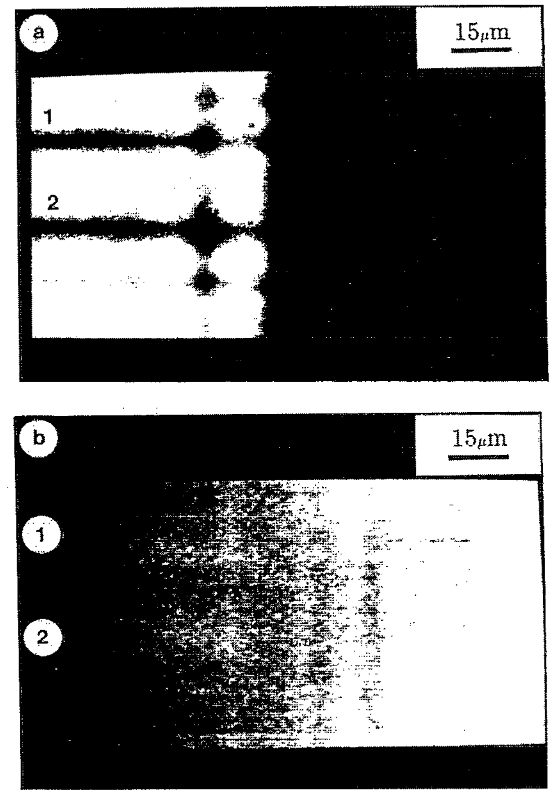

FIG. 2. CL images of the Ni-contaminated misfit dislocations, $E_0=25$ keV, $T=5$ K, $I_b \approx 1$ nA, (a) monochromatic image using Si substrate feature, (b) monochromatic image using $D2$ feature.

dislocations present. However, the presence of dislocations is established using CL imaging in a powerful indirect method. Instead of imaging the D-band luminescence, Fig. 1(a) shows a monochromatic CL of the Si substrate luminescence. Dark line features were revealed oriented along the ⟨110⟩ directions. Monochromatic line scans revealed that these dark lines were a result of a reduction of the Si substrate luminescence intensity. On inspection of exactly the same region with EBIC ($T=80$ K) it was clear that these dark line features were misfit dislocations. The corresponding EBIC image of misfit dislocations is shown in Fig. 1(b). These dark line CL features were also observed in all the samples containing dislocations, whether contaminated or as grown. On comparison with the EBIC measurements it was clear that there is a 1:1 correspondence of the recombination at the misfit dislocation as measured by EBIC with a dark line CL contrast.

The variation of the observed CL intensity occurs because the excitons are produced in the upper part of the sample structure (top 2–3 μm), then diffuse towards the Si substrate. The exciton density becomes reduced as the excitons recombine nonradiatively at the misfit dislocations. Therefore the density reaching the Si substrate is reduced and the Si CL intensity is reduced.

The dislocations in the as-received layer had no detectable room temperature EBIC contrast (detection limit $\approx 0.1\%$). It was only on cooling that the dislocations became visible with a very small contrast ($c<0.5\%$). This behavior can be attributed to shallow levels connected with misfit dislocations.[7]

The EBIC measurements showed that the contrast was nonuniform following Ni contamination. As with the as-grown sample there were regions where the dislocations could only be observed at temperatures below 300 K [identified as Ni (I)], and there were also regions where dark spots were observed at room temperature [identified as Ni (II)]. In these regions the misfit dislocations became visible at $T=250$ K. The EBIC contrast measured on these samples reached a few percent at $T=80$ K, much larger than those measured on the as-grown sample. An in-depth study has been carried out on these samples[7] and the variation of the temperature dependence of the EBIC contrast for the as-grown and Ni-contaminated [Ni (I)] can be explained by shallow levels connected with the dislocations. Shockley–Read–Hall recombination simulations show a semiquantitative agreement with the experimental results. In the areas where the dark spots were dominant [Ni (II)], the corrected contrast of these spots decreases as the sample temperature decreases. This behavior has been observed for $NiSi_2$ precipitates in FZ Si[8], and in addition transmission electron microscopy measurements have shown that Ni precipitates are observed in the Si/SiGe samples.

Figure 2(a) shows a monochromatic CL image of misfit dislocations in the Ni-contaminated sample [Ni (I)] using the Si substrate feature. Monochromatic CL imaging of the same area revealed that the $D1$ and $D2$ intensity increased at the dislocation and was also distributed between

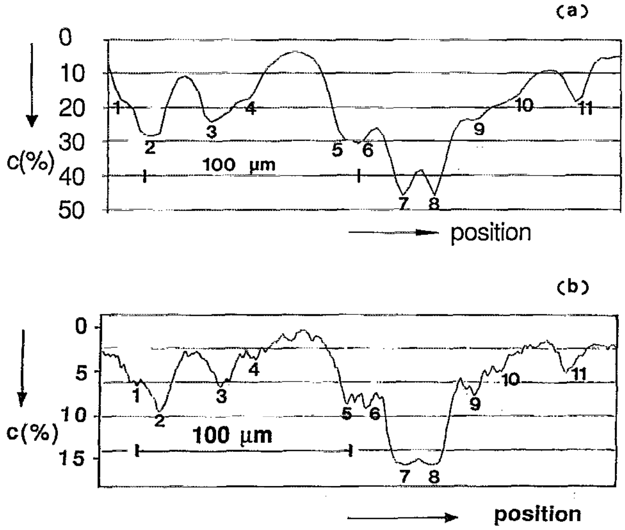

FIG. 3. EBIC and CL line scans across 11 parallel dislocations in the Ni-contaminated sample, (a) CL line scan, $E_0=25$ keV, $T=5$ K, $I_b\approx$ nA, (b) EBIC line scan, $E_0=30$ keV, $T=80$ K, $I_b\approx 0.1$ nA.

the dislocations. The monochromatic CL image using the $D2$ feature is shown in Fig. 2(b). Line scans show that the CL intensity increased by up to 15% at the dislocation. This is in contrast to the previously reported results,[4] where the $D1$ and $D2$ intensity was more dominant in between the dislocations. These differences may be due to competition for the excitons between the centers responsible for $D1$, $D2$ and $D3$, $D4$. In this study only $D1$ and $D2$ are present whereas in the previous study all four D bands were present.

CL spectra recorded on the Ni-contaminated sample contained only the $D1$ and $D2$ bands and the Si substrate features. This is in contrast to previous CL measurements on dislocations in SiGe epilayers[4] and may be due to the high temperature annealing that has destroyed or modified the structure of the centers responsible for $D3$ and $D4$.

In the strongly Ni-contaminated area of the sample [Ni (II)], monochromatic CL line scans revealed that the D-band intensity decreased by up to 30% at the dislocation. This is consistent with previous PL measurements on defects in Si, where as the level of transition metal contamination increased there was a decrease in the D-band luminescence. This was thought to be due to the microprecipitates absorbing the centers responsible for the D bands.[9] In addition, the dark line CL contrast has increased and so has the EBIC contrast. Clearly the precipitates can increase the nonradiative recombination occurring at the dislocation. The competition between nonradiative and radiative transitions for exciton capture is greatly affected by the presence of metallic impurities.

Combined CL and EBIC experiments have been routinely used to study dislocations in compound semiconductors. Such analysis allowed the simultaneous measurement of EBIC and CL contrast at dislocations and enabled comparisons to be made.[10] CL contrast is defined as $C_{CL}=(I_{CL}-I_{CLD})/I_{CL}$, where I_{CL} is the CL intensity away from the defect and I_{CLD} is the CL intensity at the defect. A similar expression can be used for the EBIC contrast (C_{EBIC}). Figure 3(a) shows the CL line scan (using the Si substrate feature) across 11 parallel dislocations [numbered in Fig. 3(a)] in the Ni-contaminated sample. The corresponding EBIC line scan over the same region is shown in Fig. 3(b). On inspection of these line scans it is clear there is a correlation in dislocation position and relative contrast. These line scans were used to determine the EBIC contrast and CL dark line contrast (using the Si substrate feature) for individual misfit dislocations, the results are summarized for all the samples in Table I. On inspection of both the EBIC and CL dark line contrast it is clear that there is a semiquantitative agreement in the relative variation of the contrast.

TABLE I. 1:1 Correlation of dislocation recombination contrast observed in CL and EBIC.

Sample	Dislocation No.	C_{CL}(%)	C_{EBIC}(%)
As grown[a]	1	<6	<0.3
As grown[a]	2	6	0.3
Ni(I)[b]	1	29	9
Ni(I)[b]	2	24	7
Ni(II)	1	5	3
Ni(II)	2	15	7

[a]Misfit dislocations numbered in Fig. 1.
[b]Misfit dislocations numbered in Fig. 2.

Although the EBIC and CL measurements were carried out under different conditions of injection level and temperature, the CL contrast measurements have not been corrected for absorption losses. It is clear that the EBIC and CL contrasts follow similar trends, with the same relative variation in contrast between different dislocations. It is feasible that the shallow centers responsible for EBIC contrast may be responsible for variations in the CL dark line contrast. These shallow levels may be introduced during growth and may result from the elastic strain field of the dislocation.[11]

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