Optical properties of treated and untreated monocrystalline p- Si<111>, p-Si<100>, n-Si<111> and n-Si<100> wafers in the visible region at room temperature

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Abstract

Silicon only based materials have dominated the electronic applications for the past few decades and now the materials have almost reached its saturation point. However there is a new great opening for silicon only based material to re-dominate consumer product market place and that is in the area of photonics. The motivation for the re-domination is driven by all silicon opto-electronics and therefore any development of silicon optical properties would hold the promise of having both electronics and optics on the same chip. Among important key ingredients for silicon technological success in photonic applications is the ability to change their refractive index and surface texture. The refractive index modification leads to the change of extraction efficiency through the change of surface roughness and material quality.

In this work, we use temperature treatment to modify optical properties and surface texture of monocrystalline p-Si<111>, p-Si<100>, n-Si<111> and n-Si<100> wafers. Optical properties of our samples were observed using both ellipsometry and PL systems and surface roughness is observed using AFM technique. The PL system used He-Ne laser operating at 543.5nm. The PL spectra were taken at room temperature in the visible region. The results showed that the treated samples have increased PL intensity and uniformity in the visible region compared to those of untreated samples. In addition the treated p-type Si samples showed better PL intensity enhancement compared to those of treated n-type samples. The explanation for this behavior will be discussed using AFM images and ellipsometry measurements.

1. Introduction

Integration and economy of scale are the two key ingredients in the technological success of silicon. Nano-structuring is an effective way to turn silicon into a photonic material. Silicon is well known as an electronic and mechanical material but it is hardly ever used as an active optoelectronic element, due to its inefficient radiative recombination from an indirect band gap[1]. Its band gap (1.12 eV) is ideal for room temperature operation, and its oxide (SiO_2) allows the processing flexibility to place more than 10^8 transistors on a single chip [2]. This yields incredible processing capability and high-speed device performance [2].

After ten years of intense research, the expectations run high that silicon can enter the field of photonics with a leading role and not only as a passive or substrate material. Many research efforts are now spent towards a silicon laser [3]. In many applications the desired optical/electrical properties are influenced by silicon surface texture. The surface roughening is an irreversible process, i.e.once the surface has become rough it is impossible to smooth it [4]. In general, a high number of structural defects change the electronic and optical properties of semiconductors. Most of defects present in silicon are detrimental to performance of devices. Internal quantum efficiency is weakened by large roughness and defects density [4-7]. Huge efforts have been undertaken in order to minimize defects in crystal growth and devices processing. Also the surface roughness and defects should be minimized to ensure the mechanical strength of microstructures, uniform device performance

Reduction the absorption and scattering of the silicon light emission due to defects and inhomogeneities is required to reach the photonics applications pretension.

The carrier lifetime that depends on recombination rate and excess hole/electron concentration is determined by the fundamental properties of material, as well as by the defects present [7]. It is an essential parameter in determining the main features of an electro-optic device [7].

Surface recombination effects are becoming progressively more important as silicon semiconductor device dimensions are reduced, as well as it is more important than bulk recombination processes [7, 8].

Two factors contribute to the surface energy: first, the density of dangling bonds, and secondly the surface stress. Surface stress is generated when the surface atoms re-bond to reduce the number of dangling bonds. Both factors depend on the orientation of surface. The surfaces with lowest numbers of dangling bonds per surface area will have the lowest surface energy and consequently be the most stable surfaces [9]. The Si <111> surface shows the lowest surface energy because the Si-Si bonds in the bulk are all directed along one of the <111> directions. The reconstruction of Si <100> has widely been studied because of its technological importance and as Si <100> surfaces in reality generally show a small miscut to the desired orientation [9].

Silicon nano-particles showed visible light emissions from 5000 Å to 9000 Å, with peak intensity at 8000-8200 Å, when excited with a He-Cd laser.

The PL intensity increased with decreasing particle size [10]. The PL for particles larger than 9 nm is surface state-induced, while the PL for those smaller than 9 nm is ascribed to quantum confinement (QC) effects [2, 10].

PL spectra show a continuous shift of peak energy from the Si bulk band gap to the visible region (as in porous silicon) with a good agreement with QC effect [10]. Quantum confinement of carriers in nano-structured materials leads to a high quantum efficiency of the radiative recombination as well as to increase of the optical band gap, so the PL originates from transitions between the band edges [12].

The existence of the dangling bonds on the surface results in various surface states deep in the Si energy gap; these states have a direct energy gap and yield visible luminescence [12]. These effects open the possibility of light emitting devices in the visible region [12].

In this work, we use temperature treatment to modify optical properties and surface texture of monocrystalline p-Si<111>, p-Si<100>, n-Si<111> and n-Si<100> wafers. We have studied the optical properties of treated and untreated monocrystalline p-Si<111>, p-Si<100>, n-Si<111> and n-Si<100> wafers using spectroscopic ellipsometry (SE), atomic force microscopy (AFM) and photoluminescence (PL).

2. Experimental Procedure

Temperature treatment has been carried out on mono-crystalline silicon wafers subjected to ultra cooling temperature treatment, where all the samples are subjected to the same treatment time. To ensure optimal interaction between laser source and the sample especially during PL measurement, all the samples were coated with silver as a back surface reflector. In this work three different techniques are used to characterize the properties of untreated and treated silicon samples, namely AFM, ellipsometry and PL.

The AFM is ideal for quantitatively measuring the nanometer scale surface roughness and visualizing the surface nano-texture on many types of materials surfaces. This nondestructive technique provides a very high three dimensional spatial resolution. In this work we used AFM Surface Imaging System operating with laser at 780nm. Spectroscopic ellipsometry is a non-destructive optical technique based on measurement of the change in light polarization upon reflection from a sample surface or interface which in turn is due to the change in refractive index. This work used Gaertner ellipsometry operating with 632.8nm laser light.

As for the PL, we have used a home made system using CW He-Ne laser operating at 543.5nm as an excitation source. For PL measurements, laser beam was focused on the sample using a lens with 15cm focusing length. Different incidence laser beam angles, in the range of 0^0-75^0 with respect to the normal, have been used. The sample was mounted on a rotational disk with a scalar from 0^o to 90^o angle. Emitted signal from the sample was collimated before entering monochromator slit to ensure a good collection of the emission signal from the samples. All the measurements were made at room temperature at atmospheric pressure.

3. Result and Discussions

Figures (1a-1b) and figures (1c-1d) show the AFM images of untreated and treated n-Si with <100> and <111> orientations respectively. The images indicate that the temperature treatment has changed the surface texture of both orientations. The treatment has essentially improved the surface quality of samples n-Si<100> and n-Si<111>. Figures (2a-2b) and figures (2c-2d) show the AFM images of untreated and treated p-Si with <100> and <111> orientations respectively. Similarly the temperature treatment has improved the surface quality of samples p-Si<100> and p-Si<111>. Sample p-Si<111> however displays less noticeable difference in surface texture.

Figure 3 shows ellipsometry results for n-Si<100> sample before and after the treatment. There is noticeable difference in refractive index between samples before and after the treatment especially at higher angle of incidence. The average refractive index value before the treatment is about 3.8 and increases to about 3.81 after the treatment. Figure 4 shows the results for n-Si<111> sample before and after the treatment. No significant change of refractive index in this sample is observed as a result of the treatment. The average refractive index value before the treatment is about 3.81. A closer look into this figure reveals that the treatment has reduced slightly the average refractive index value.

Figure 5 shows ellipsometry results for wafer p-Si<100> before and after the treatment. Unlike n-type samples there is a significant change of the refractive index due to the treatment in this sample. The refractive index has increased from average 3.7 before the treatment to an average of about 3.82 after the treatment. Figure 6 shows the results for wafer p-<111> before and after the treatment. Again a significant change is also observed in this sample. The treatment has increased the average refractive index from 3.63 to about 3.81. From ellipsometry results in figures 3, 4, 5 and 6, it is obvious that refractive index of p-type Si samples experience more noticeable change compared with those of n-type Si samples. It is also interesting to note that the value of about 3.8 seems to be the 'stable' refractive index value for all Si samples. This means that if before the treatment, a Si sample having slightly higher value than the 'stable' value, the treatment will slightly reduce the value as in the case of samples n-Si<111> (figure 4). Similarly if before the treatment, a Si sample having lower value than the 'stable' refractive index value, the treatment will increase it to the 'stable' value as in the case of samples n-Si<100> (figure 3), p-Si<100> (figure 5) and p-Si<111> (figure 6). Unlike AFM results which reveal the surface morphology, the ellipsometry results reveal surface as well as bulk properties. The change in refractive index value implies the changes in the bulk properties of the samples. Since p-type samples displayed significant changes in refractive index value in responding to the treatment, it is interesting to study further the optical properties of these samples. For this reason, further discussion will focus on p-type Si wafers.

Photoluminescence spectroscopy is a spontaneous emission of light from a material under optical excitation which can be used to characterize a variety of material parameters, such as information on the quality of surface, interfaces and in the bulk. Figure 7a and figure 7b show PL spectra in the visible region from 550nm to 850nm for p-Si<100> before and after the treatment respectively. It is evident from these figures that the PL peaks and intensity were influenced by the treatment. Figure 8a and 8b show PL spectra for p-Si<111> before and after the treatment respectively. Again similar effect is observed in this sample as what have been observed in sample p-Si<100>. The PL results for both samples are consistent with the ellipsometry results in that the treatment has changed their optical properties. The consistent results from different characterization techniques could be explained by the fact that PL spectrum is about the production of free carriers after the interaction of the sample with incident light (i.e. laser). These free carriers can then recombine at the surface or in the bulk to give photoluminescence. The thermalization of carriers is not exclusively radiative [7] and non-radiative recombination may occur through successive emission of phonons. Radiative and non-radiative rate depend on the fundamental properties of the materials (i.e. bandgap and refractive index) and the defects present. These parameters in turn affect the generation of free carrier concentration when sample is incident by light.

Since we have changed the fundamental properties of the sample (i.e. surface texture and refractive index), so does the generation of free carriers and hence the PL emission.

Note from figures 7b and 8b that both types of sample exhibit a smoother PL spectrum as a result of the treatment. Further, both samples exhibit increased overall PL intensity in this region (i.e. 550nm – 850nm) with blue shift in PL peaks around red emission (~625nm). The results are very interesting in that one can modify and enhanced the PL properties of p-type silicon wafer. Despite interesting, these results demand explanations. One plausible explanation for this behavior is by using quantum confinement effect of the nano-crystal, *nc*. The p-type samples could be treated as a bulk medium comprising of *nc* structures with different sizes. The rough PL spectrum in the visible region for both samples before the treatment could originate from *nc*s with a large variety of different sizes and from defect centers. However, after the treatment the smoother PL spectrum suggests that the distribution of *nc* sizes is more balanced from one size to another or maybe due to some of the defect centers have been removed due to the treatment. After the treatment the majority of the nc sizes fall within this emission range (550nm to 850nm). This could explain the overall increased PL intensity after the treatment. The blue shift around ~625nm suggests that some *nc* have their size decreased [2,12]. It is also noticeable from figure 7 and figure 8 that PL intensity for p-Si<111> is higher than for p-Si<100>. Also figure 8b reveals that enhancement of PL from p-Si<111> after the treatment is more than that observed from p-Si<100> in figure 7b. This is explained by lower surface energy in p-Si<111> [9].

4. Conclusions

We have shown that using ultra cooling temperature treatment one can modify the surface properties and optical properties of silicon wafers. The temperature treatment has essentially improved surface quality of all the samples studied in this work.

We also found that refractive index of all the silicon samples can be modified with the treatment despite small change from n-type silicon. After the treatment we found that the 'stable' refractive index value for all the samples is in the average of about 3.8. The treatment time was the same for all the samples. There is a possibility that n-type silicon requires different treatment time than p-type to observe significant change in refractive index value. In optoelectronics devices, this capability of modifying optical characteristics means controlling of photons propagations, the transitions between the energy levels and quantum efficiency. The PL results on the treated p-type silicon presented in this work have shown overall improvement of the spectrum. This is quite a satisfactory results taking into account that all PL measurements were conducted at room temperature and at atmospheric pressure. The change in PL emission after the treatment is consistent with the change in refractive index value. Finally, the capability to modify the optical properties of crystalline silicon will lead to better understanding of Si-based material in the pursuit of making high performance photonic devices.

5. Acknowledgement

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6. References

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Figure caption

Figure 1. AFM images of Si samples a) untreated n-Si<100> b) treated n-Si<100> c) untreated n-Si<111> and d) treated n-Si<111>.

Figure 2. AFM images of Si samples a) untreated p-Si<100> b) treated p-Si<100> c) untreated p-Si<111> and d) treated p-Si<111>.

Figure 3. Refractive index of n-Si<100> before and after the treatment

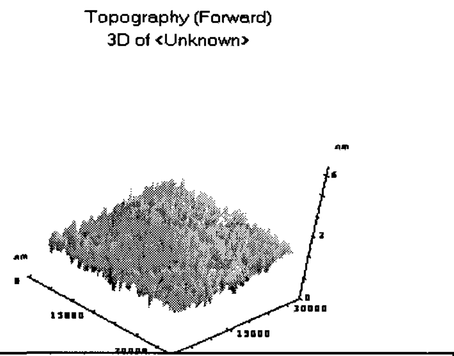
Figure 4. Refractive index of n-Si<111> before and after the treatment.

Figure 5. Refractive index of p-Si<100> before and after the treatment

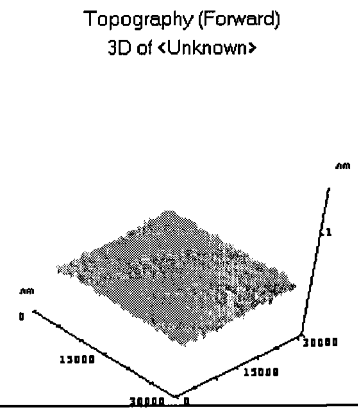
Figure 6. Refractive index of p-Si<111> before and after the treatment.

Figure 7. PL spectrum in the visible region for p-Si<100>: a) before temperature treatment, b) after temperature treatment.

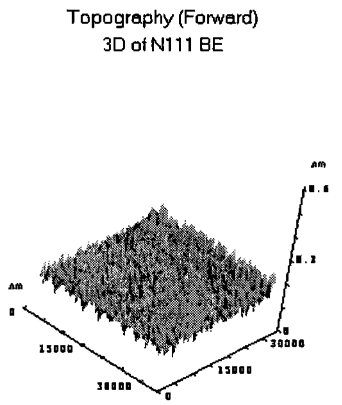
Figure 8. PL spectrum in the visible region for p-Si<111> : a) before temperature treatment, b) after temperature treatment.



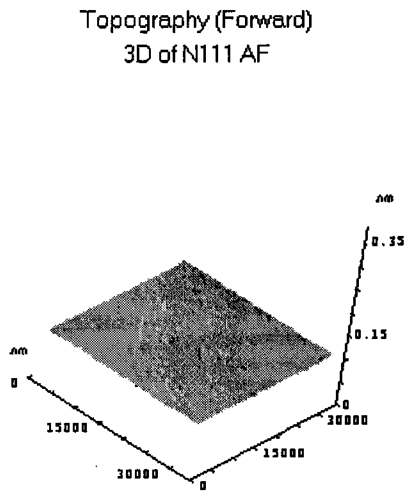
a) n-Si<100> before treatment



b) n-Si<100> after treatment

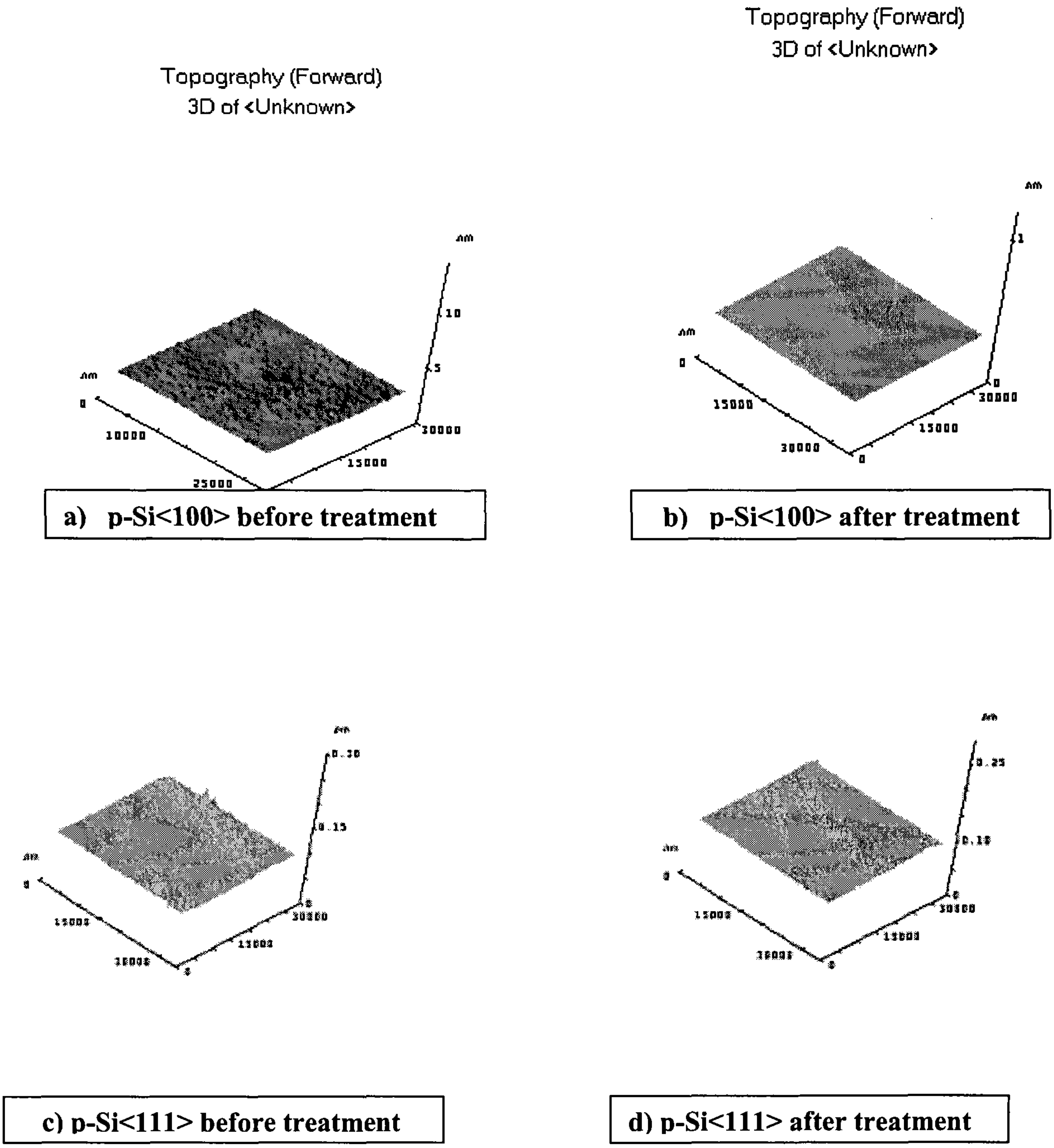


c) n-Si<111> before treatment



d) n-Si<111> after treatment

Figure 1



a) p-Si<100> before treatment

b) p-Si<100> after treatment

c) p-Si<111> before treatment

d) p-Si<111> after treatment

Figure 2

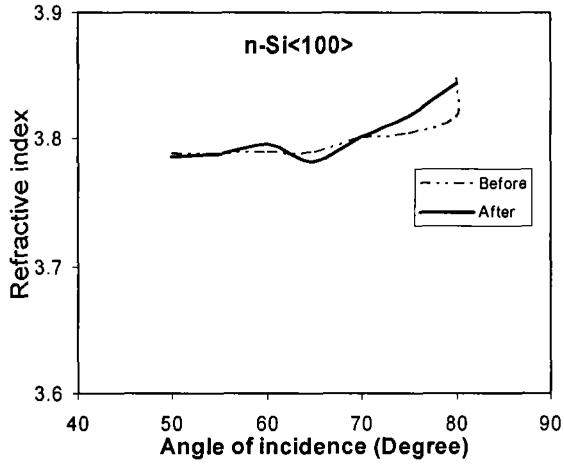
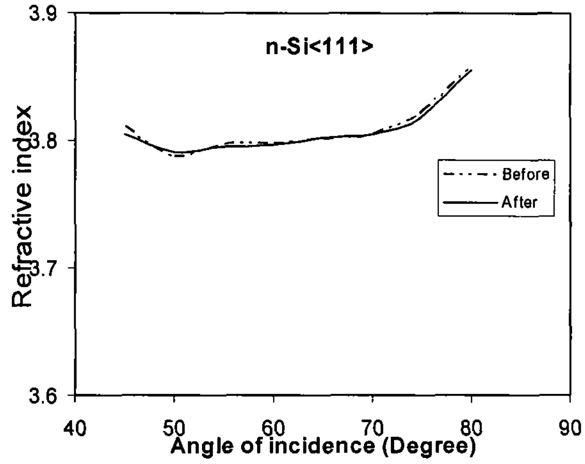

n-Si<100>
Refractive index
Angle of incidence (Degree)
Before
After
3.9
3.8
3.7
3.6
40
50
60
70
80
90

Figure 3



n-Si<111>
Refractive index
Angle of incidence (Degree)
Before
After
3.9
3.8
3.7
3.6
40
50
60
70
80
90

Figure 4

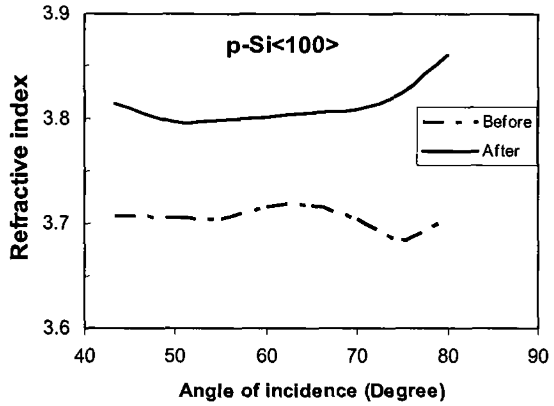

p-Si<100>
Refractive index
3.9
3.8
3.7
3.6
40
50
60
70
80
90
Angle of incidence (Degree)
Before
After

Figure 5

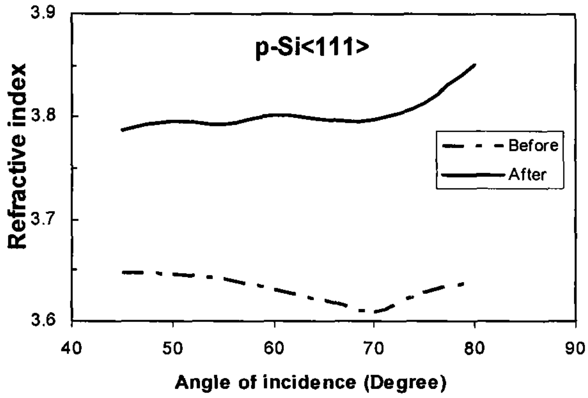

p-Si<111>
Refractive index
3.9
3.8
3.7
3.6
40
50
60
70
80
90
Angle of incidence (Degree)
Before
After

Figure 6

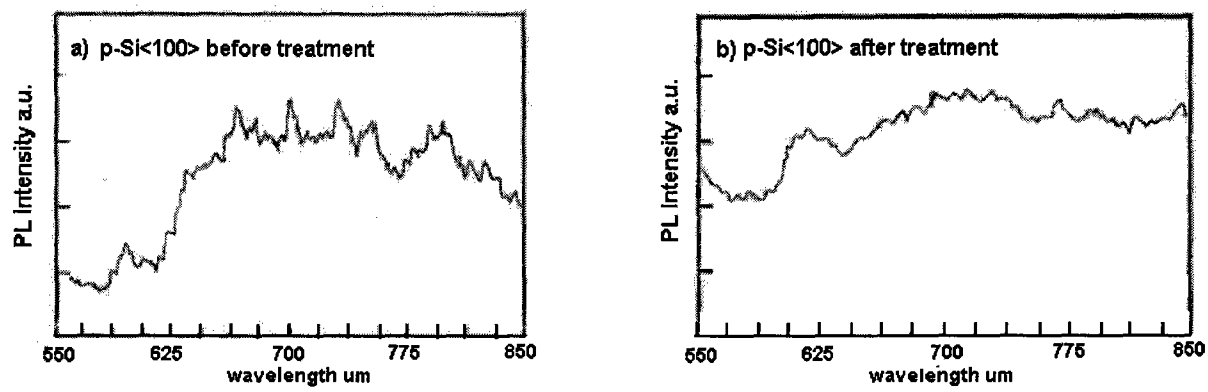

a) p-Si<100> before treatment
PL Intensity a.u.
550
625
700
775
850
wavelength um
b) p-Si<100> after treatment
PL Intensity a.u.
550
625
700
775
850
wavelength um

Figure 7

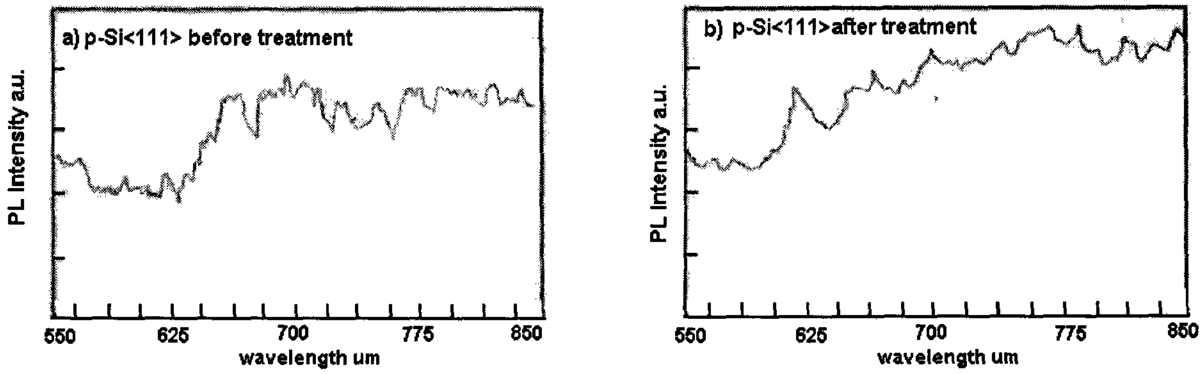

a) p-Si<111> before treatment
PL Intensity a.u.
550
625
700
775
850
wavelength um
b) p-Si<111>after treatment
PL Intensity a.u.
550
625
700
775
850
wavelength um

Figure 8