Nitrogen-doped Silicon: Mechanical, Transport and Electrical Properties

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A novel dislocation locking technique is used to study the behaviour of nitrogen in float-zone silicon (FZ-Si). Specimens containing well-defined arrays of dislocation half-loops are subjected to isothermal anneals of controlled duration, during which nitrogen diffuses to the dislocations. The stress required to bring about dislocation motion is then measured. From measuring this unlocking stress as a function of annealing time and temperature it is possible to deduce information on nitrogen transport and nitrogen-dislocation interactions. In this paper, the results obtained by using the dislocation locking technique are reviewed. Furthermore, deep-level transient spectroscopy (DLTS) and high-resolution DLTS (HR-DLTS) are applied to nitrogen-doped silicon. A deep-level with an emission enthalpy of approximately 0.50eV and a concentration of order 10^{11}cm^{-3} was found in n-type nitrogen-doped FZ-Si and n-type nitrogen-doped neutron transmutation doped FZ-Si. No additional deep-levels with a concentration of greater than 6 x 10^{10}cm^{-3} were found in either material. No deep-levels were found in p-type nitrogen-doped Czochralski silicon (Cz-Si), for which the detection limit was approximately 10^{12}cm^{-3}.

Introduction

Manufacturers of silicon wafers have recently become interested in intentionally adding nitrogen to wafers as it provides flexibility in controlling oxygen precipitation in Czochralski silicon (Cz-Si) [1-5], controls vacancy concentration [6] and improves mechanical strength [7-12]. In spite of its utility, many of the fundamental properties of nitrogen in silicon, such as its diffusivity, transport mechanism, binding energy to dislocations and electrical activity, remain a matter of debate.

The majority of nitrogen in silicon exists in the form of dimers [13] and it has been established that nitrogen dimers are interstitial defects [14]. Numerical simulations generally suggest that the nitrogen atoms in the dimer are strongly bound with an energy of 3.67 to 4.30eV [15-17] and that the dimer is practically immobile with an activation energy for diffusion of 2.38 to 2.69eV [18,19]. Experimental data obtained from a SIMS out-diffusion investigation give an activation energy for nitrogen transport as 2.8eV in the 800 to 1200ºC temperature range [20]. However, nitrogen diffusion in nitrogenimplanted silicon has been shown to exhibit anomalous behaviour [21,22], indicating that the transport of nitrogen is not a simple problem. Recently, it has been proposed that nitrogen is transported by a dissociative mechanism, whereby a practically immobile nitrogen dimer splits into two monomers which diffuse with an activation energy of 1.38eV and then recombine [23]. However, because of the insensitivity of SIMS to nitrogen in silicon, measurements of nitrogen transport are limited to date and so alternative methods of measuring transport should be considered.

Dislocations in materials can be pinned by impurity atoms and the critical resolved shear stress necessary to move these locked dislocations is known as the *unlocking stress*. By studying the variation in the dislocation unlocking stress as a function of annealing time at different temperatures, it is possible to deduce information on impurity transport and impurity-dislocation interactions [9,12,24-27]. Such a dislocation locking technique has been used to study oxygen in Cz-Si, for which it reproduced existing values obtained by SIMS for the diffusivity of oxygen in the 700 to 850ºC temperature range [24] and provided new evidence for enhanced oxygen transport due to dimer diffusion in the 350 to 650ºC temperature range [25,26]. Results obtained by using the technique also provide evidence for enhanced oxygen diffusion in Cz-Si with a high concentration of boron [27].

Float-zone silicon (FZ-Si), which is virtually free of impurities such as oxygen, acts as a model system for the study of other impurities in silicon. The dislocation locking technique has been applied to nitrogen-doped FZ-Si with different nitrogen concentrations [9,12]. Data which show the variation of the dislocation unlocking stress with annealing time at annealing temperatures from 500 to 1200ºC are reviewed. Additionally, data are reviewed which show, for given annealing conditions, the dependence of dislocation unlocking stress on unlocking temperature in the 500 to 700ºC temperature range. By making a small change to the standard dislocation locking technique [9, 24-27], it is possible to obtain a measurement of impurity out-diffusion. Results using this method are presented which show out-diffusion of nitrogen from FZ-Si annealed for 15 hours at 750°C.

A standard technique for the study of electrically active defects in semiconductors is deep-level transient spectroscopy (DLTS) [28]. Authors of several experimental studies using DLTS have attributed electrically active defects in silicon to nitrogen [29-32]. The results of the older studies [29,30] should be treated with caution as the silicon available at the time was of a significantly lower standard than it is today. More recent studies suggest that nitrogen results in levels at E_c - 0.42eV [31], E_c - 0.5eV [32] and E_v + 0.55eV [32], with the level at E_c - 0.5eV also being found in older work [30]. The electrical activity of nitrogen-related defects has also been investigated theoretically by the use of density-functional theory calculations [17]. In this work, DLTS and the related technique of high-resolution DLTS (HR-DLTS) [33,34] are used to obtain new experimental results on the electrical activity of nitrogen-related defects in silicon.

Neutron transmutation-doped (NTD) FZ-Si is used in applications for which little resistivity variation across the wafer is required, such as for high power devices. The material is produced by bombarding conventionally-grown FZ-Si with neutrons, which induces a nuclear reaction in which some silicon atoms are converted to phosphorus atoms. Resistivity shifts of 5 to 10% can occur during subsequent annealing schedules of nitrogen-doped NTD FZ-Si [35] and it is possible that if a nitrogen-related defect is responsible for this then it will be observed in DLTS experiments. In this work, DLTS and HR-DLTS are also applied to as-grown nitrogen-doped NTD FZ-Si.

Experimental Methods

Dislocation Locking Technique

For the standard dislocation locking experiments, FZ-Si wafers produced by Topsil Semiconductor Materials A/S were used. Bars measuring 2mm by 1mm by 30mm were cleaved from a (111) wafer (220Ωcm n-type) with a nitrogen concentration of 2.2×10^{15} cm^{-3} and bars measuring 0.5mm by 3.5mm by 30mm were cleaved from a (100) wafer (>10,000Ωcm p-type) with a nitrogen concentration of $3 \times 10^{14} cm^{-3}$. The nitrogen concentrations were determined using FTIR carried out by the manufacturer. For the out-diffusion experiments, a (100) nitrogen-doped FZ-Si wafer (>100Ωcm) produced by Wacker was cleaved into bars measuring 0.55mm by 3.5mm by 30mm. The nitrogen concentration in the wafer was measured to be $2.5 \times 10^{15} cm^{-3}$ by FTIR carried out by the manufacturer. It should be noted that since there is no generally accepted calibration standard for nitrogen concentrations in silicon, the nitrogen concentrations measured by the different manufacturers cannot be directly compared.

A Vickers diamond tip was used with a 0.1N load and a 5s dwell time to place indents at 250μm intervals along the length of each bar. The bars were then subjected to a four-point bend at temperatures between 400 and 600ºC to grow the punched-out dislocation half-loops to a diameter of 100 to 200μm. Specimens with the lower nitrogen concentration and those used in the out-diffusion experiments were cooled to below 400ºC before the load was removed.

For the standard dislocation locking experiments, the bars were then annealed at constant temperatures (from 500 to 1200ºC) for various times (from 0 to 4345 hours). Specimens annealed at temperatures of 1000ºC and lower were annealed in argon atmosphere. Specimens annealed at 1100ºC and 1200ºC were sealed in evacuated silica ampules and were quenched after annealing by placing the ampule directly into water. In this way it is thought that no significant dislocation locking occurred during cooling. A planar etch comprising HF (40%), HNO_3 (69%) and CH_3COOH (glacial) in the ratio 8:75:17, which was found to etch silicon at the rate of approximately 0.8μm per minute at room temperature, was used to remove a controlled amount of material from each bar after annealing. For the standard dislocation locking experiments, the amount of material removed was 30μm for specimens annealed below 1000ºC and 50μm for specimens annealed at 1000ºC and above. This was done to remove the damage associated with the indents and to negate the effects of nitrogen out-diffusion.

A three-point bend at elevated temperature was then applied to each specimen. The stress in a three-point bending configuration varies linearly from the outer to the central knife-edges. Thus, dislocation half-loops at different points along the bar were subjected to different stresses [24]. A preferential etch comprising CrO_3 (0.3M) and HF (40%) mixed in the ratio 5:4 was then used to reveal the dislocation half-loops. Optical microscopy was used to locate the dislocation half-loop that moved under the least resolved shear stress (*i.e.* the unlocking stress).

For most measurements the temperature of the three-point bending process was carefully controlled to be 550ºC. However, for one set of experiments the temperature dependence of the unlocking process was also investigated. Sets of specimens with a nitrogen concentration of 3 x 10^{14}cm^{-3} were annealed at the same temperature for a fixed time (640ºC for 150 hours and 700ºC for 50 hours). These specimens were then subjected to a three-point bend at different temperatures in the 500 to 700ºC temperature range.

To measure nitrogen out-diffusion, a small modification to the standard dislocation locking technique was made. A set of dislocation-containing nitrogen-doped FZ-Si specimens was produced using the methods described above. The specimens were all then annealed at 750ºC for 15 hours. After this annealing stage, a different amount of material was removed from each specimen by the planar etch; from 5 to 55µm. This was instead of the 30 or 50µm of material removed in the standard process. The dislocation unlocking process was carried out by three-point bending at 550ºC.

DLTS and HR-DLTS

DLTS [28] and HR-DLTS [33,34] were used to investigate nitrogen-doped silicon. The properties of the materials investigated in this work are summarised in Table 1. The FZ-Si was supplied by Topsil Semiconductor Materials A/S and the Cz-Si was supplied by MEMC Electronic Materials Inc.. Circular Schottky diodes with a diameter of 1mm were formed on the polished surface of the specimens. Gold Schottky contacts were evaporated onto n-type silicon specimens and titanium Schottky contacts were sputtered onto p-type silicon specimens. Aluminium Ohmic contacts were evaporated onto the unpolished side of all specimens.

Specimen	**[N] [cm^{-3}]**	**[O] [cm^{-3}]**	**Type (dopant)**	**Carrier concentration [cm^{-3}]**
FZ-Si	7 x 10^{14}	< 10^{16}	n (phosphorus)	2 x 10^{13}
NTD FZ-Si	~ 10^{15}	< 10^{16}	n (phosphorus)	3 x 10^{13}
High [N] Cz-Si	2.1 x 10^{15}	5.74 x 10^{17}	p (boron)	1 x 10^{15}
Low [N] Cz-Si	1.0 x 10^{15}	5.82 x 10^{17}	p (boron)	7 x 10^{14}

Table 1. The properties of the nitrogen-doped silicon investigated by DLTS and HR-DLTS in this work. Oxygen concentrations are stated to the DIN 50438/I standard.

For all specimens investigated, DLTS and HR-DLTS were carried out with a reverse bias of -7V and a 1ms fill pulse of -2V. For HR-DLTS, the FLOG algorithm [34] was used to analyse the data. For all HR-DLTS experiments, the sampling rate was chosen to be 60kHz, 7,000 scans were made and 9,000 data samples were taken for each scan. All DLTS data were taken as the sample heated up.

Results

Dislocation Unlocking Measurements

The dislocation unlocking stress measured at 550ºC as a function of annealing time at different annealing temperatures is shown in Figure 1. Data at other temperatures for high nitrogen-containing specimens have been published elsewhere [9]. Nitrogen is found to provide a strong locking effect on dislocations in FZ-Si for annealing temperatures from 500 to 1200ºC.

The unlocking stress as a function of annealing time exhibits two distinct regimes for both nitrogen concentrations investigated. In the first regime the unlocking stress rises approximately linearly with annealing time, at a rate which is dependent on the annealing temperature and on the specimen's nitrogen concentration. In the second regime the unlocking stress takes a constant value, which is dependent on the nitrogen concentration and is approximately independent of the annealing temperature. For annealing temperatures of 1000ºC and above, data were only obtained in the second regime. This is because with the present experimental configuration the duration of the first regime is too short to allow accurate measurements to be obtained.

The gradient of the initial rise in unlocking stress, τ_u, with annealing time, t, in the first regime can be used to deduce the activation energy for the dislocation locking process. The rate of the initial rise in unlocking stress, $\frac{d\tau_u}{dt}$, is plotted as a function of reciprocal temperature in Figure 2. This gives the activation energy of the dislocation locking process to be 1.5 ± 0.1eV for both concentrations of nitrogen.

The unlocking stress measured as a function of unlocking temperature in the 500 to 700ºC temperature range for specimens subjected to certain annealing conditions is shown in Figure 3. It can be seen that the unlocking stress decreases approximately linearly with increasing unlocking temperature.

In Figure 4, the unlocking stress measured at 550ºC is plotted as a function of the material removed from specimens subjected to anneals at 750ºC for 15 hours. The unlocking stress increases with the amount of material removed, before reaching an approximately constant value of 65MPa.

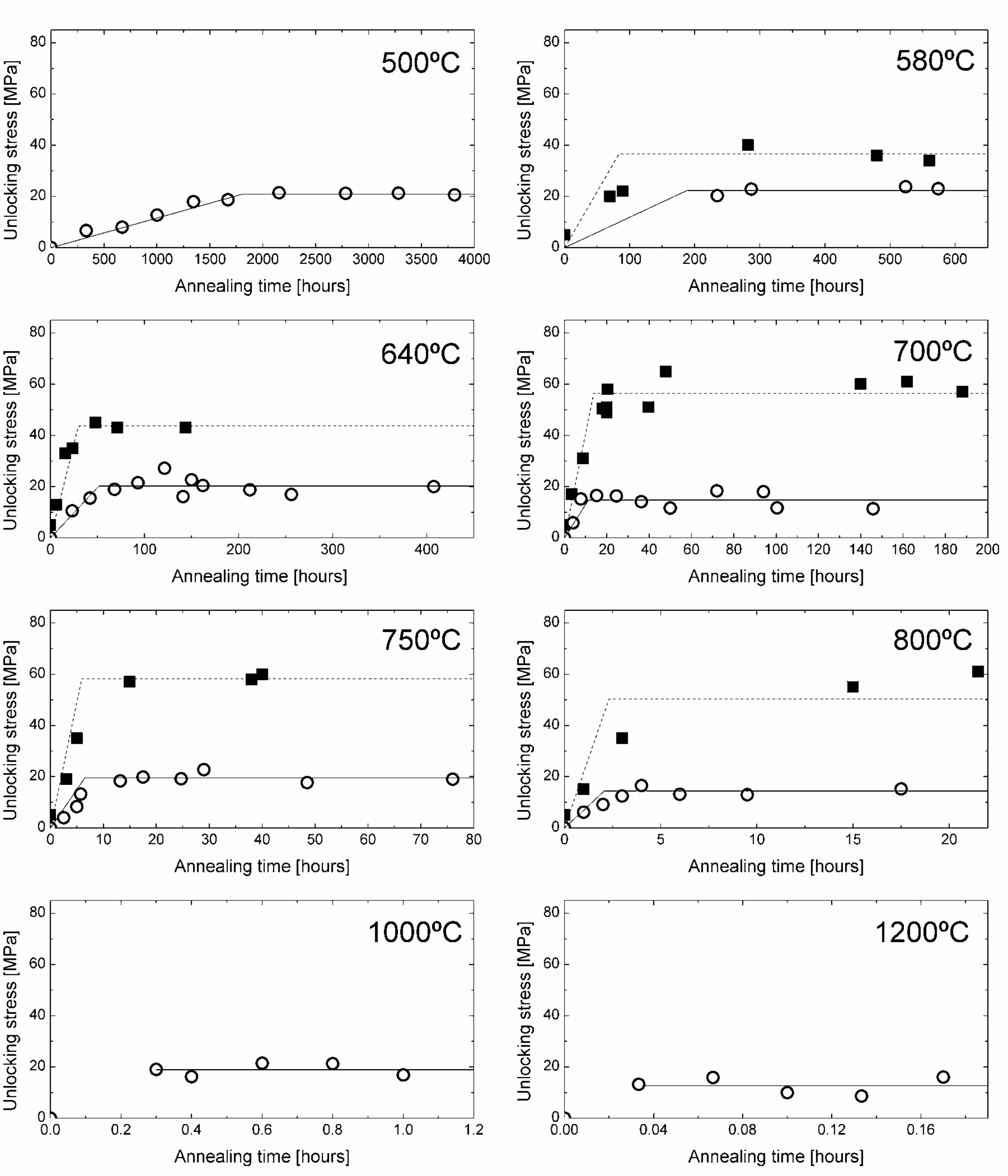

Figure 1. The dislocation unlocking stress measured at 550ºC as a function of annealing time at selected annealing temperatures. The closed squares are for nitrogen-doped FZ-Si with a nitrogen concentration of 2.2 x 10^{15}cm^{-3} and the open circles are for nitrogen-doped FZ-Si with a nitrogen concentration of 3 x 10^{14}cm^{-3}.

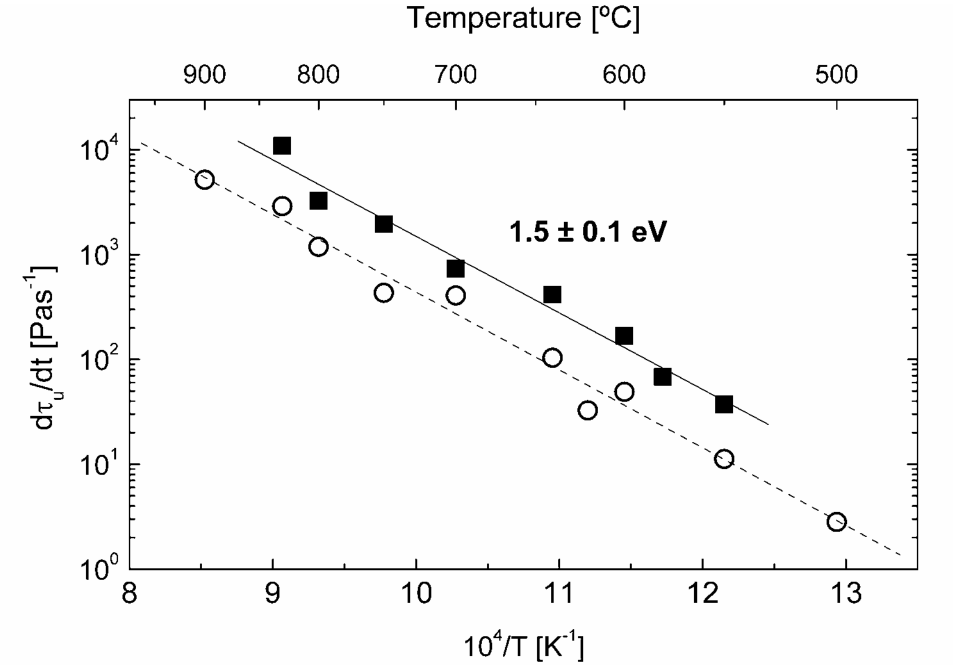

Figure 2. An Arrhenius plot of the gradient of the initial rise in unlocking stress (regime 1), $\frac{d\tau_u}{dt}$, for specimens annealed at temperatures from 500ºC and 900ºC. The symbols used are the same as those in Figure 1. Best fit lines to each set of data points are shown, both of correspond to an activation energy of 1.5 ± 0.1 eV.

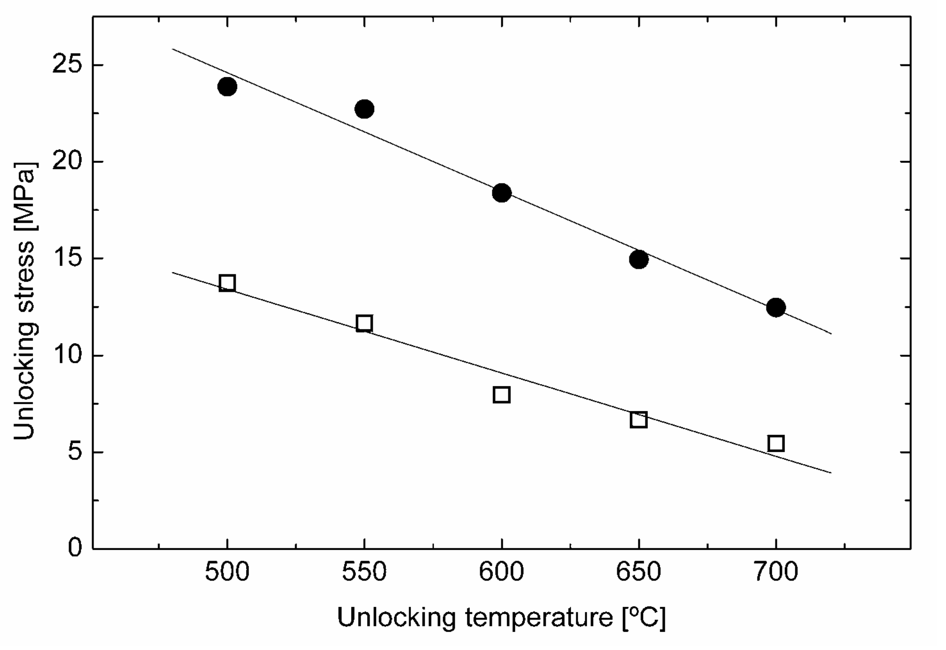

Figure 3. The dependence of the dislocation unlocking stress on unlocking temperature for nitrogen-doped FZ-Si with a nitrogen concentration of 3 x $10^{14}cm^{-3}$. The filled circles represent dislocation unlocking stresses in specimens annealed at 640ºC for 150 hours. The open squares represent unlocking stresses measured on dislocations locked by annealing at 700ºC for 50 hours.

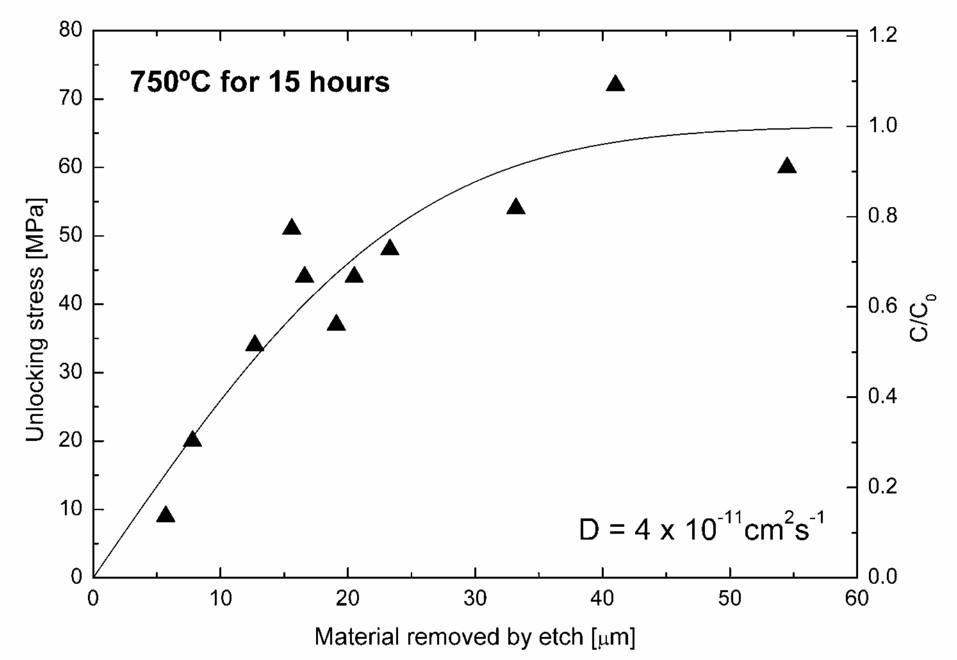

Figure 4. The dislocation unlocking stress in nitrogen doped FZ-Si with a nitrogen concentration of $2.5\text{x}10^{15}\text{cm}^{-3}$ measured as a function of material etched away, *x*, after annealing at 750°C for 15 hours. The closed triangles represent unlocking stress measurements. The curve is an error function of the form $\frac{C}{C_0} = \text{erf}\left(\frac{x}{\sqrt{Dt}}\right)$, where C/C_0 is the nitrogen concentration as a proportion of the total nitrogen concentration, *D* is the effective diffusivity of nitrogen and *t* is the annealing time.

DLTS and HR-DLTS Measurements

Nitrogen-doped FZ-Si. DLTS was performed on nitrogen-doped FZ-Si in the 67 to 320K temperature range with six rate windows, ranging from 4 to 200s^{-1}. The DLTS spectra obtained for some of these rate windows are shown in Figure 5. A single peak was found, which was located at 283K for a 200s^{-1} emission rate. The height of the peak was approximately 0.03pF, implying a trap concentration of approximately 3 x 10^{11}cm^{-3}.

HR-DLTS was then used to determine the emission rate at eleven different temperatures in the 250 to 270K temperature range. The HR-DLTS spectra showed just one peak, indicating that the peak found in the conventional DLTS spectra is associated with a single defect state. From the variation of emission rate with temperature, the activation enthalpy was deduced from the HR-DLTS data to be 0.50 ± 0.01eV, as shown in the Arrhenius plot in Figure 5. The capture cross-section of the trap was found to be greater than 5 x 10^{-14}cm^2.

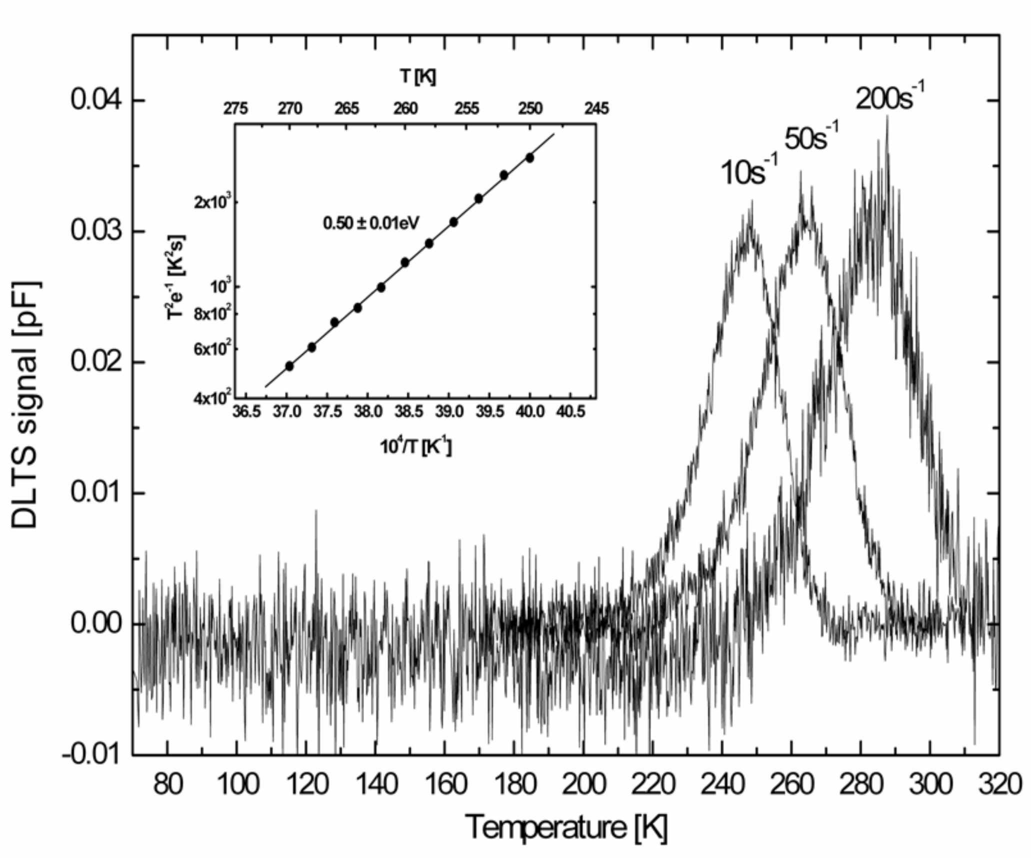

Figure 5. DLTS spectra for nitrogen-doped NTD FZ-Si taken with selected rate windows. Also shown in the Figure is the Arrhenius plot used to deduce the activation enthalpy of the trap from the HR-DLTS data.

Nitrogen-doped NTD FZ-Si. DLTS was performed on nitrogen-doped FZ-Si in the 67 to 320K temperature range. Data were taken at six different rate windows in the 4 to 200s^{-1} range. The DLTS spectrum taken with a 50s^{-1} rate window is shown in Figure 6. A single peak was found for all rate windows investigated. The temperature at which the peak occurred was 289K for a 200s^{-1} rate window. The height of the peak was approximately 0.01pF, implying a trap concentration of approximately 1 x 10^{11}cm^{-3}.

HR-DLTS was then used to determine the emission rate from the trap at eleven temperatures in the 250 to 270K temperature range. Again, the HR-DLTS spectra showed just one peak, indicating that the peak found in the conventional DLTS spectra is associated with a single defect state. From the variation of emission rate with temperature, the activation enthalpy was deduced from the HR-DLTS data to be 0.49 ± 0.01eV, as shown in the Arrhenius plot in Figure 6. The capture cross-section of the trap was found to be greater than 8 x 10^{-14}cm^{2}.

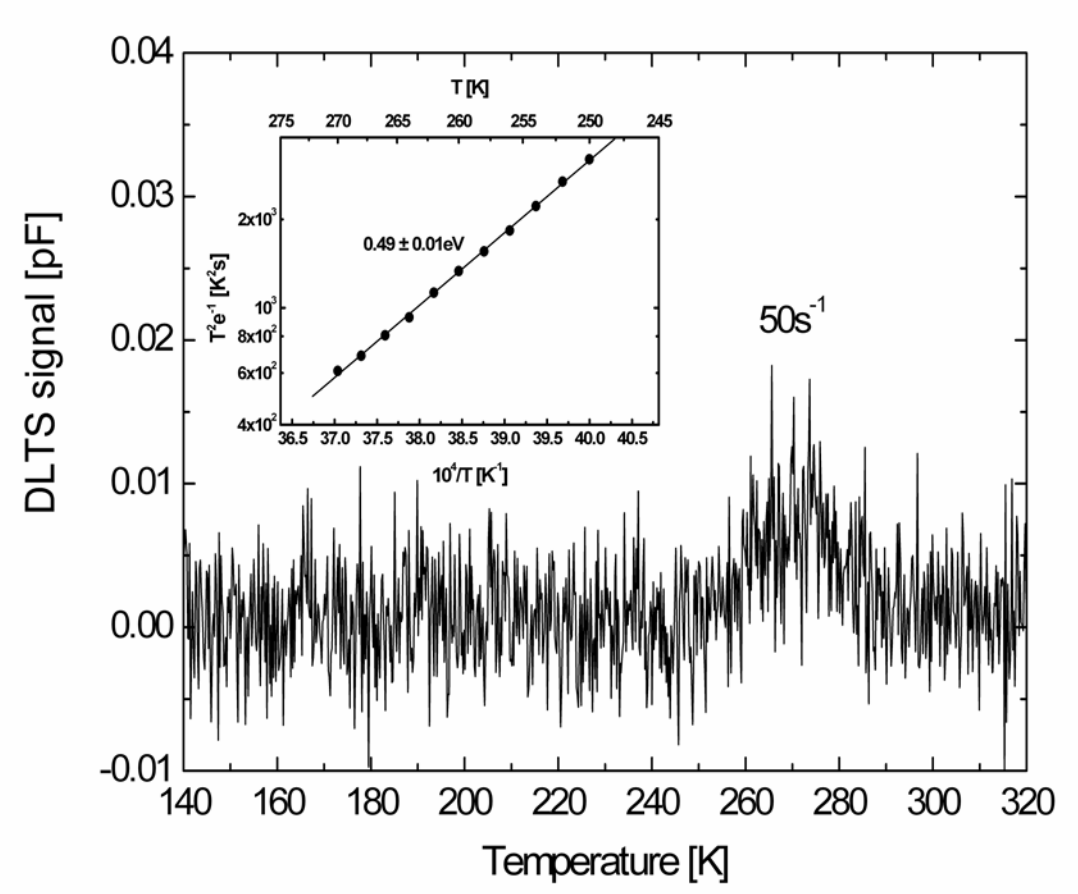

Figure 6. DLTS spectrum for nitrogen-doped NTD FZ-Si taken with a $50s^{-1}$ rate window. Also shown in the Figure is the Arrhenius plot used to deduce the activation enthalpy of the trap from the HR-DLTS data.

Nitrogen-doped Cz-Si. DLTS was performed at temperatures from 67 to 320K with rate windows of 80 and $200s^{-1}$. No peaks were found in the Cz-Si with the high nitrogen concentration or in the Cz-Si with the low nitrogen concentration. The noise level for the high nitrogen-containing Cz-Si was typically of order 0.01pF, which corresponds to a detection limit of approximately $10^{12}cm^{-3}$.

Discussion

Mechanical and Transport Properties

It has been shown in this work that nitrogen is capable of providing a strong locking effect on dislocations, even though it is present in a concentration of just 3 x $10^{14}cm^{-3}$ in some specimens. The dislocation unlocking stress measured at 550ºC has been found to be significant for specimens annealed at temperatures up to at least 1200ºC.

The fact that dislocation locking by nitrogen is stable up to 1200ºC suggests that nitrogen binds strongly to the dislocation core. In previous work it was shown that dislocation locking by oxygen in Cz-Si is strongly reduced at temperatures greater than approximately 800ºC [24], as above this temperature oxygen, which has a binding energy to the dislocation core of 0.74eV, "boils off" the dislocation. Thus, the present work shows that nitrogen impurities provide dislocation locking in FZ-Si after annealing at temperatures at which oxygen impurities in Cz-Si do not lock dislocations. It is suggested that the addition of nitrogen to Cz-Si would be beneficial for the mechanical properties of these wafers, as nitrogen may be able to immobilise dislocations at temperatures at which the locking due to oxygen is practically non-existent.

From the Arrhenius plot in Figure 2, the activation energy for the dislocation locking process has been found to be approximately 1.5eV for both concentrations of nitrogen. The stress required to unpin the dislocation from nitrogen is also thermally activated. For the particular sets of annealing conditions studied, the unlocking stress decreases approximately linearly with the temperature at which the unlocking process takes place. Previous work using the same technique for oxygen in Cz-Si also shows an approximately linear dependence of dislocation unlocking stress on unlocking temperature [26].

If it is assumed that nitrogen diffuses to the specimen's surface during the annealing process, then a nitrogen concentration profile will be produced. Therefore, upon annealing, the segments of the dislocations close to the specimen's surface experience a nitrogen concentration lower than those in the bulk and will consequently be less strongly locked. During the subsequent unlocking process, the dislocations will first unpin from the position at which they are locked least strongly and it is this value of the unlocking stress that is measured. Thus, by removing different thicknesses of material after the annealing stage, the strength of the dislocation pinning at different depths beneath the surface, which depends on the nitrogen concentration at that depth, can be measured. In this work, 5 to 55μm of material was etched away from the surface of a set of dislocation-containing specimens annealed at 750ºC for 15 hours. As shown in Figure 4, the dislocation unlocking stress measured in these specimens was found to increase as more material was removed, before it reached an approximately constant value.

The data are only indicative of the nitrogen concentration profile in the specimen since the concentration profile evolves during the course of the anneal. However, they do give an indication of the distances over which nitrogen diffusion to the surface is occurring. Bearing in mind these limitations, an error function profile fitted to the data in Figure 4 gives the diffusion coefficient of nitrogen in silicon at 750ºC to be approximately $4 \times 10^{-11}\text{cm}^2\text{s}^{-1}$. The nitrogen out-diffusion measured by the dislocation locking technique is consistent with that expected from a SIMS investigation by Itoh and Abe, since extrapolation of their reported diffusion expression gives a value of $4.3 \times 10^{-11}\text{cm}^2\text{s}^{-1}$ at this temperature [20].

Electrical Properties

A deep-level with a concentration of approximately $3 \times 10^{11}\text{cm}^{-3}$ with enthalpy of 0.50 ± 0.01eV was found in nitrogen-doped FZ-Si with a nitrogen concentration of $7 \times 10^{14}\text{cm}^{-3}$. The trap was found to have a capture cross-section of greater than $5 \times 10^{-14}\text{cm}^2$.

To a good approximation the trap found in this work can be considered to be located at 0.50eV below the conduction band, *i.e.* at E_c – 0.50eV. A trap at E_c – 0.50eV has previously been observed in DLTS experiments on FZ-Si doped with nitrogen during growth by Nauka *et al.* [30] and on silicon into which nitrogen had been in-diffused by Kakumoto and Takano [32]. In the work of Nauka *et al.* the trap was not observed in as-grown nitrogen-doped FZ-Si, but was found to appear in a concentration of 4 x 10^{-11}cm^{-3} after annealing at 900°C for 3 hours [30]. In the work of Kakumoto and Takano the trap concentration was found to depend on the in-diffused nitrogen concentration and was found to exist in concentrations of 7 x 10^{13}cm^{-3} and lower [32]. Kakumoto and Takano measured the capture cross-section of the trap to be 7.6 x 10^{-16}cm^{2}. The results presented in this paper are the first to show that the E_c – 0.50eV trap exists in untreated FZ-Si doped with nitrogen during growth. However, it is noted that the lower limit on the capture cross-section obtained in this work is inconsistent with the value measured by Kakumoto and Takano [32].

No other deep-levels were observed in the present work. Other deep-levels have been observed in DLTS experiments on n-type nitrogen-doped silicon at E_c – 0.19eV [29,30], E_c – 0.28eV [29,30], E_c – 0.42eV [31] and E_c – 0.58eV [30]. The traps at E_c – 0.19eV and E_c – 0.28eV were observed in as-grown FZ-Si doped with nitrogen during growth. The studies in which these levels were found were conducted by Tokumaru *et al.* [29] and Nauka *et al.* [30] and they were published in 1982 and 1985 respectively. It is possible that the traps they observed were in fact nitrogen-related, but with the vast improvements in silicon technology that have occurred in the past twenty years or so, that these defects no longer exist in detectable concentrations in as-grown material. The deep-levels at E_c – 0.42eV and E_c – 0.58eV were only found to occur after annealing [30,31]. Thus, it is likely that these traps do not exist in as-grown material, which is why they were not observed in this work.

A deep-level with concentration of approximately 1 x 10^{11}cm^{-3} and enthalpy of 0.49 ± 0.01eV was found in nitrogen-doped NTD FZ-Si with a nitrogen concentration of order 10^{15}cm^{-3}. The trap was found to have a capture cross-section of greater than 8 x 10^{-14}cm^{2}. Within experimental error, the enthalpy of this trap is the same as the trap observed in nitrogen-doped FZ-Si which had been electrically doped by conventional means. The trap concentration is a factor of three less than that in the conventionally-doped material. However, it should be noted that the nitrogen concentration in the NTD material is only estimated from the growth conditions and it is possible that the nitrogen concentration could be significantly lower than 10^{15}cm^{-3}. This deep-level, which can be considered to be located at E_c – 0.49 ± 0.01eV, was the only deep-level found in nitrogen-doped NTD FZ-Si. This therefore suggests that either the neutron bombardment process itself creates no electrically active defects in a concentration detectable with the experimental configuration used with the specimens available, or that any electrically active defect produced combines with nitrogen to produce an electrically inactive complex. The noise of the DLTS spectra for nitrogen-doped NTD FZ-Si, such as that presented in Figure 6, is typically 0.005pF. Thus, an upper limit can be put on the concentration of electrically active defects related to neutron bombardment at approximately 6 x 10^{10}cm^{-3}.

The concentration of the deep-level found at approximately E_c – 0.50eV in this work suggests that approximately 1 in every 2,000 nitrogen atoms form part of an electrically active defect. From the experimental results presented in this paper alone it is not possible to identify the precise structure of the deep-level observed. Kakumoto and Takano, who also found a defect with the same enthalpy, suggest that the defect is a N_2-vacancy complex [32]. They deduced that dimeric nitrogen was part of the defect as the diffusivity of nitrogen as deduced from their DLTS study was consistent with a SIMS out-diffusion study by Itoh and Abe [20], which concluded that nitrogen dimers were lost to the surface. Additionally, in their work Kakumoto and Takano found that the concentration of the deep-level was decreased by injection of silicon interstitials from an oxide layer, so they deduced that vacancies were part of the defect. The results of *ab initio* calculations may offer some insight into the structure of the defect found in this thesis. Calculations by Goss *et al.* predict a level at E_c – 0.50eV due to the N_sV defect [17]. It is possible that N_sV is responsible for the deep-level observed in this work.

The DLTS results for p-type nitrogen-doped Cz-Si showed no deep-levels. A previous study by Kakumoto and Takano found a deep-level at E_v + 0.55eV in p-type Cz-Si into which nitrogen had been in-diffused [32]. This defect was not observed in this present work, but this may simply be because its concentration is less than the detection limit of approximately 10^{12}cm^{-3}.

Conclusions

Dislocation locking by nitrogen in FZ-Si has been investigated in the 500 to 1200ºC temperature range. It has been shown that nitrogen, despite being present at a concentration of only 3 x 10^{14}cm^{-3} in some specimens, is effective at locking dislocations across this wide temperature range. It is noted that dislocation locking by nitrogen in FZ-Si is stronger than that due to oxygen in Cz-Si at high temperatures (> 800ºC) and it is suggested that the addition of nitrogen to Cz-Si will improve its mechanical properties.

The dislocation locking by nitrogen as a function of annealing time at a particular temperature is found to have two distinct regimes. By analysing the first regime, a linear rise, it is possible to deduce the activation energy for the dislocation locking process as 1.5eV. The release of a dislocation from nitrogen impurities has also been shown to be a thermally activated process in the 500 to 700ºC temperature range.

The dislocation unlocking stress has been measured in a set of nitrogen-doped FZ-Si specimens annealed at 750ºC for 15 hours, each of which has had a different amount of material removed from its surface after the annealing stage. The dislocation unlocking stress is found to increase with material removed, until it takes an approximately constant value. This variation in dislocation locking is due to nitrogen out-diffusion. From fitting an error function profile to the experimental data, the diffusion coefficient of nitrogen in silicon is deduced to be approximately 4 x 10^{-11}cm^{2}s^{-1} at 750ºC.

The results presented in this paper show that a deep-level in a concentration of order 10^{11}cm^{-3} with an enthalpy of approximately 0.50eV exists in n-type nitrogen-doped FZ-Si and n-type nitrogen-doped NTD FZ-Si. The capture cross-section of the trap is greater than 5 x 10^{-14}cm^2. The state is attributed to a nitrogen-related defect. A trap with the same activation enthalpy has previously been found in annealed nitrogen-doped FZ-Si [30] and silicon into which nitrogen had been diffused [32]. The results presented in this work are the first to show the trap in as-grown material. No evidence was found for neutron-transmutation doping creating any extra defects in the FZ-Si studied, for which the detection limit was approximately 6 x 10^{10}cm^{-3}. No deep-levels were found in p-type nitrogen-doped Cz-Si, for which the detection limit was of order 10^{12}cm^{-3}.

Acknowledgments

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