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# Complexes defects induced by neutron irradiation of Cz-silicon

**Nadjet Osmani[1] · A. Cheriet[2]**

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## Abstract

The boron-doped Cz-Si was irradiated with 1 MeV neutrons delivered by the Es-Salam reactor at two different neutron fluence values, $1.98\times10^{18}$ and $3.96\times10^{18}$ n/cm$^2$, respectively. Annealing processes were carried out under argon atmosphere, at 550 °C and 950 °C for 60 min, respectively. The effects of isochronal annealing on the neutron-irradiated silicon's IR absorption spectrum are presented. The obtained results indicate two forms of the Near-Edge Absorption that increase with increasing neutron fluence. One centered at 1000–1500 nm (NEA-1) and second near 1600–1800 nm (NEA-2). After the annealing process at 550 °C, the IR absorption spectrum shows the change of the first Near-Edge Absorption band towards a shorter wavelength at 1000–1200 nm range as well as the disappearance of the (NEA-2) band near 1800 nm. The appearance of the lithium impurity associated with divacancy at 1700 nm that confirms the transmutation of boron into lithium of the samples. At 950 °C, the experimental data show that 1700 nm which is associated with Li divacancy persists for higher neutron fluence, but not for lower fluence.


**Keywords** Neutron fluences · Silicon · Defects · UV–Vis–NIR spectrophotometer

## 1 Introduction

Silicon neutron transmutation doping (NTD) method used modern technology and nanotechnology as a perfect semiconductor doping [1–5]. However, during NTD processes, the fast neutron and gamma ray introduces defects in silicon crystals. The most important interest of NTD process, high doping accuracy and homogeneity of phosphorus, was not immediately realized commercially; however, attempts were made utilize the excellent doping control inherent in the process to fabricate high resistivity detectors and integrated circuit as early as 1964 [6]. It is important to know the various modifications in defect distribution of the silicon crystal derived with neutron irradiation for developed electronic instrument manipulating in radioactive environments [7]. Damage in the crystal arising from structural defects, internal electric fields, etc., will cause a complex defects [8] as divacancies, interstitials, and impurity atoms out or the sharp edges in the electronic density states at the valence and conduction bands. Associated electronic absorption under the interdict band is then obvious and has been named near-edge absorption (NEA) [9]. Therefore, a research of the (NEA) band in neutron-irradiated silicon gives some knowledge on the defect complexes. Additional development of irradiation-resistant solar cells for space applications and in particle detectors for high-energy physics experiments needs more information about the generation mechanisms and the properties of irradiation produced point defects [10]. Consequently, the mechanism of defects after neutron irradiation of Cz-Si has been studied in the previous works [11–14]. Londos [15] have explained that a great divacancy concentration ($V_2$) is present after neutron irradiation of silicon; it corresponds to the 1800 nm band. An energy level below the conduction band corresponded to the 1800 nm band and that this absorption band might not be observed if the level is occupied by electrons [9]. Displacements of lattice atoms are observed when silicon samples are irradiated with high neutron fluence [16, 17]. Divacancies and other clusters are created in dense displacement regions where migration of the defects is involved. They take position following the primary generation of silicon interstitial (I) and vacancies (V) in the crystal lattice [18]. The study of boron-doped Cz-Si by NTD gives more information about complex defects such as

✉ Nadjet Osmani
osmaninadjet@yahoo.fr

[1] Nuclear Research Center of Birine, BP 180, 17200 Ain Oussera, Djelfa, Algeria

[2] Research Center for Semiconductor Technology Energetic, 2 Bd Frantz Fanon Alger, BP no 140, 7 , 16000 Merveilles, Algeria

the vacancies and divacancies associated with lithium impurity atoms. Following the study of Young et al., on the behavior of defects created in silicon by irradiation through identifying the defects associated with Lithium atoms. They assumed that 1400 and 1700 nm due to the complex consisting of one or two Lithium ions, respectively, are trapped by the divacancy [19]. Lithium's major technical applications in semiconductors are focused on their interaction with the other defects. Lithium, which is highly mobile in silicon at ambient temperatures, can serve as an electrically active donor unless it is precipitated and can interact with other impurities, existing defects, and irradiation defects to form additional donors [20, 21]. The capture of thermal neutrons by the boron-10 excites the $^{10}$B to an unstable $^{11}$B state, which undergoes fission into high-energy alpha particles (helium nuclei) and high-energy nuclei of lithium-7. These experimental results explained by the following the nuclear reaction [22]:

$$^{10}\mathrm{B}\ +^{1}\mathrm{n} \rightarrow^{11}\mathrm{B}^{*} \rightarrow^{7}\mathrm{Li}^{*} +^{4}\mathrm{He} \rightarrow^{7}\mathrm{Li} +^{4}\mathrm{He}\ + \gamma\ (480\ \mathrm{keV}). \tag{1}$$

Furthermore, all these defects introduce deep and shallow levels in the interdict band and affect on electrical properties such as the mobility of charge carriers in Si-based devices [23]. Simultaneously, the changes in the XRD, Raman, AFM, the substrate resistivity, and photoluminescence of the boron-doped Cz-Silicon samples have been studied before the previous work [24]. Others studies have indicated that heat treatment is required to remove lattice damage in Cz-Si NTD [25]. Therefore, this study is a continuation of our work reported in Ref [24], and the main goal of this study is to assess the complexes defects of silicon, generated by neutron irradiation using UV–Vis–NIR spectrophotometer technique. In fact, essential information was achieved using optical characterization of neutron irradiation and annealed boron-doped CZ-Si.

## 2 Experimental study

In this study, the boron-doped Cz-Si wafer was purchased from "Thin Films and Surfaces" laboratory from France. Their initial oxygen and carbon concentrations were small than $10^{18}$ and $10^{16}$ cm$^{-3}$, respectively. The irradiated process for the samples, with 1 MeV neutrons at a temperature of 50 °C, was performed in the heavy water moderator of the Es-Salam research reactor under two neutron fluences of $1.98\times10^{18}$ and $3.96\times10^{18}$ n/cm$^2$. The nuclear reactions of Cz-silicon is as follows:

$$^{30}\mathrm{Si}\ (\mathrm{n},\gamma)^{31}\mathrm{Si} \rightarrow^{31}\mathrm{P}\ \left(T_{1/2} = 2.6\ \mathrm{h}\right). \tag{2}$$

This is based on the capture of thermal neutron by $^{30}$Si to create phosphorus $^{31}$P. The neutron energy spectrum of the reactor was obtained as previously mentioned [26]. Isochronal annealing (60 min) was carried out at 550 °C and 950 °C in a quartz tube furnace under argon atmosphere. We choose this temperature according to the work of Londos [27], where they assume the appearance of $V_nO_m$ defects at 550 °C, and oxygen precipitate at 950 °C annealing, respectively [28]. The optical characterization of the samples has been investigated at room temperature (RT) using the ultraviolet–visible–near-infrared (UV–Vis–NIR) spectrophotometer (Varian Cary 500).

## 3 Results and discussion

Figure 1 shows the IR absorption spectrum in the 1000–1900 nm wavelength range for the boron-doped Cz-Si, before and after irradiation at two neutron fluences. An absorption band at 1800 nm appears after irradiation at two neutron fluence values. Fan and Ramads suggested that the 1800 nm absorption band is related to $V_2$ divacancies corresponding to electron transition illustrating an excited state [9]. In addition, the spectrum contains two forms of the near-edge absorption bands, which increase with increasing neutron fluence. The first one centered in 1000–1500 nm wavelength range (NEA-1) which observed in Refs. [29–32]. The second one near-edge absorption band (NEA-2) was in the 1600–1800 nm wavelength range. It should be noted that these two kinds of Near-Edge Absorption band are not present in the spectrum before irradiation.

In our previous work [24], we concluded from Raman spectroscopy that there is no systematic influence of the

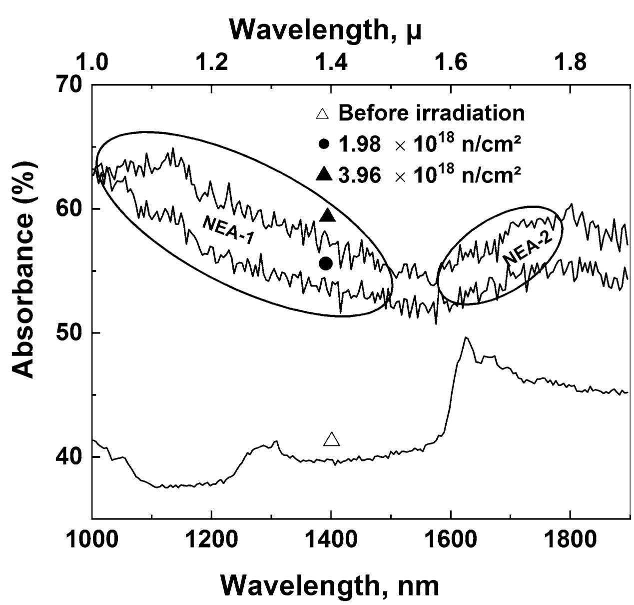


**Fig. 1** IR absorption spectrum of boron-doped Cz-Si before irradiation (unfilled triangle) and after neutron irradiation at fluence values of $1.98\times10^{18}$ n/cm$^2$ (filled circle) and $3.96\times10^{18}$ n/cm$^2$ (filled triangle)

neutron fluence on the crystallinity of the boron-doped Cz-silicon. Figure 2 shows a typical spectrum for boron-doped Cz-Si after irradiation at two neutron fluences and annealing at 550 °C for 60 min. After heating at 550 °C, we observe a disappearance of divacancy accompanied by the disappearance of the (NEA-2) nearby the divacancy. At the same time, the effects of thermal annealing induce displacement of (NEA-1) in the direction of short wavelengths from 1000–1500 nm to 1000–1200 nm. This shift may be attributable to the presence of an irradiated silicon absorption band in the wavelength range of 1100–1700 nm. However, it is difficult to determine this shift quantitatively. It has been shown that lithium interacts with divacancy when the annealing temperature exceeds 550 °C. The mechanism of interaction of lithium with the defects depends on the diffusion of a positively charged lithium ions, as a donor, into the initial damage site complex as follows: (Li–V–V. …) that was explained and illustrated by Faith [33]:

$$Li^{+} + V + 2e^{-} \rightarrow Li - V \tag{3}$$

$$Li^{+} + Li - V^{-} \rightarrow Li - V - Li. \tag{4}$$

Therefore, the lithium has an important effect on the kind of the near-edge absorption and his interaction with radiation-induced defects. This fact suggests that these shifts are due to the change in the energy-band curvature at a high concentration of the main impurity atoms (lithium and oxygen). The decreasing in the Near-Edge Absorption indicates a significant reduction in the crystal disorder and the introduction of additional Li donors during annealing. On the other hand, the disappearance of the near-edge absorption band at 1600–1800 nm wavelength range gives rise to the new two bands at 1400 nm and 1700 nm, and such bands can be related to one or more divacancies associated with the lithium atom. The experimental results indicate that lithium comes from the transmutation of boron from the initial samples (boron-doped Cz-Si). The same result agreed with the reported data taken by Young et al., in lithium-diffused into silicon irradiated with electrons [19]. As illustrated in Fig. 3, at higher fluence and after annealing at 950 °C (for 60 min), a significant concentration of the lithium impurity associated with divacancy 1700 nm remained and has an appreciable contribution to the donor concentration. This result was confirmed by our previous work [24] where the resistivity decreases by the interaction of $Li^{+}$ ions with divacancy.

## 4 Conclusion

In the current study, the activity of defects caused by the rapid neutron irradiation of the boron-doped Cz-Si material subjected to subsequent thermal annealing was illustrated.

The obtained results indicate two forms of the near-edge absorption which increase with increasing neutron fluence. Concerning the annealing behavior of the irradiated boron-doped Cz-Si, it was observed that the lithium appeared by fission of boron. The first NEA-1 related to

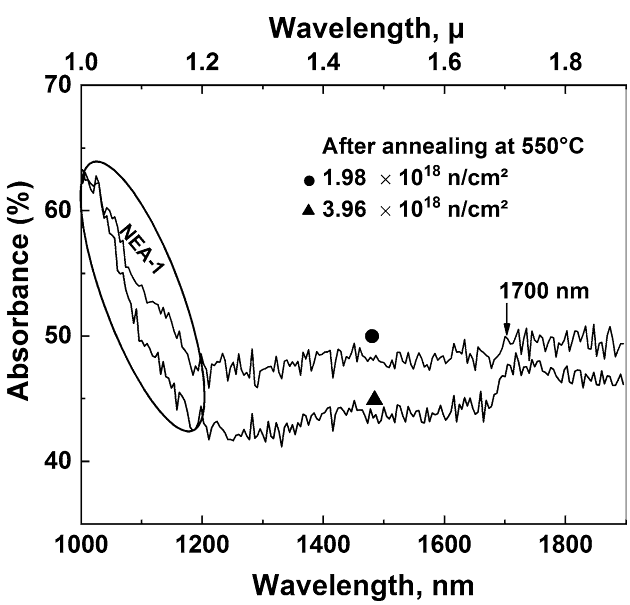


**Fig. 2** IR absorption spectrum of boron-doped Cz-Si irradiated at $1.98 \times 10^{18}$ (filled circle) and $3.96 \times 10^{18}$ n/cm$^{2}$ (filled triangle) and after isochronal annealing at 550 °C

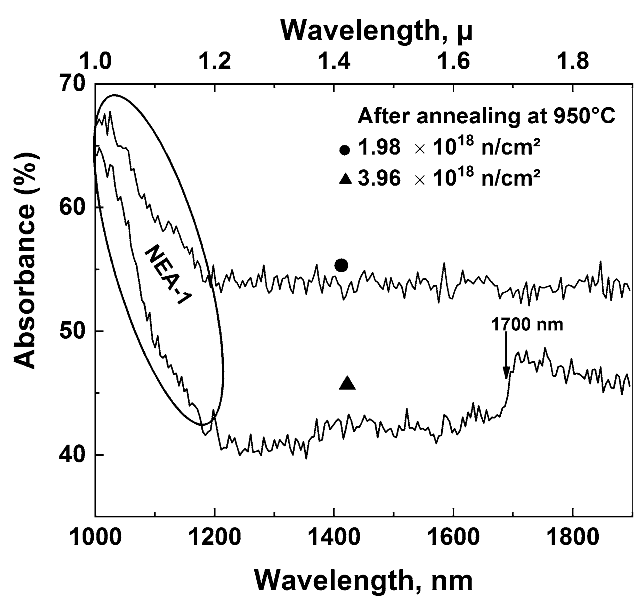


**Fig. 3** IR absorption spectrum of boron-doped Cz-Si irradiated at $1.98 \times 10^{18}$ (filled circle) and $3.96 \times 10^{18}$ n/cm$^{2}$ (filled triangle) and after isochronal annealing at 950 °C

divacancy disappears after thermal annealing at 550 °C, and the appearance of a new band at 1700 nm associated to Li divacancy. Therefore, lithium has an important effect on the formation of near-edge absorption. Finally, after annealing at 950 °C, the 1700 nm related to Li divacancy remains for higher fluence, but not for lower fluence where it not persist, these can be investigated in future works.

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