# Deep-level transient spectroscopy study of the *E* center in *n*-Si and partially relaxed *n*-$Si_{0.9}Ge_{0.1}$ alloy layers

M. Mamor,* M. Elzain, K. Bouziane, and S. H. Al Harthi
*Physics Department, College of Science, Sultan Qaboos University, P.O. Box 36 Muscat 123, Sultanate of Oman*
(Received 25 June 2007; revised manuscript received 17 October 2007; published 30 January 2008)

We have employed deep-level transient spectroscopy to investigate the electronic properties of defects introduced during high energy He-ion irradiation of epitaxially grown phosphorous-doped *n*-Si and partially relaxed *n*-$Si_{0.9}Ge_{0.1}$. It is found that He-ion irradiation introduces two major defects in Si and $Si_{0.9}Ge_{0.1}$. These have been attributed to a doubly negative charge state of the divacancy ($V_2^{=/-}$) and *V*-P pair (*E* center). The germanium dependence of the activation enthalpy ($E_H$) for both ($V_2^{=/-}$) and *V*-P pair is found to be relatively minute with a small decrease and increase in the corresponding $E_H$ with respect to that of Si, respectively. Comparison was made with earlier reported results in phosphorous-doped fully strained *n*-$Si_{1-x}Ge_x$ and antimony-doped totally relaxed *n*-$Si_{1-x}Ge_x$ layers to directly assess the influence of strain relaxation on radiation-related deep levels in $Si_{1-x}Ge_x$. It is shown that the energy level of the *V*-P pair in fully strained and partially relaxed $Si_{1-x}Ge_x$ lies closely to that reported for *V*-Sb in fully relaxed $Si_{1-x}Ge_x$. This result indicates that the *V*-P level is independent of strain, suggesting that such defect is pinned to the conduction band. Moreover, our calculation using full-potential linearized augmented plane wave method shows nonpreferential site occupancy of the phosphorous relative to Ge atoms. This implies a chemical disorder in the vicinity of the *V*-P center which leads to a fluctuation of the ionization energy level of the *E* center. This fluctuation is associated with a distribution of the electron emission rate between the *V*-P level and the conduction band edge.

DOI: 10.1103/PhysRevB.77.035213 PACS number(s): 61.72.J−, 68.55.Ln, 61.72.uf, 68.35.Dv

## I. INTRODUCTION

$Si_{1-x}Ge_x$/Si heterostructure has generated considerable interest because of its great potential applications in electronic and optoelectronic devices. The decrease in the band gap of $Si_{1-x}Ge_x$ layer with increasing either Ge content or strain in $Si_{1-x}Ge_x$ layer for a given Ge content with respect to that in Si has opened the realization of large heterostructures entirely compatible with Si integrated circuit technology (see Ref. 1 for more details). The successful technological application of such $Si_{1-x}Ge_x$/Si heterostructures based on electronic devices depends on the presence of defects and requires an extremely deep understanding of the electronic features of these defects upon alloying and strain effect. These defects affect the electrical and optical properties of the $Si_{1-x}Ge_x$ layer and the characteristics of the devices fabricated on it.[2,3] The point defects are interesting from both fundamental and technological points of view and are often associated with interstitials and vacancies as well as their association with impurities contained in the materials. One of the useful tools to introduce point defects is by using ion irradiation (electrons, protons or He ions, etc.). For instance, the vacancy-donor pair (*V* donor or *E* center), the vacancy-oxygen (*V*-O), and the divacancy ($V_2$) are the most dominant defects induced in *n*-type Si by ion irradiation with high energy particles. The structure and electronic properties of the above defects in Si are well understood.[4–6] The electronic properties of the various *E* centers in silicon, depending on the type of the doping involved, have been reported and the level position below the conduction band ranges from 0.40 for the *V*-Sb to 0.45 for *V*-P center.[7–9] In $Si_{1-x}Ge_x$ layer, the effect of composition and strain on electronic properties of divacancy $V_2$ and a vacancy-donor complex has become possible to investigate due to the ability to grow epitaxial layers with extremely low defect concentrations. The substitutional incorporation of Ge into pseudomorphic $Si_{1-x}Ge_x$ epilayer on Si has two effects on the band gap of the alloy. First, the larger size of Ge atoms relative to Si will enhance the strain in the film, thus decreasing the band gap. Second, for relaxed $Si_{1-x}Ge_x$ alloy, the intrinsic effect of Ge substitution on the energy band gap can be separately studied. Actually, both alloying and strain can coexist in the $Si_{1-x}Ge_x$ epilayer. Hence, it is possible to study how the position of the vacancy-related energy levels changes due to the change in the band structure by varying either the Ge content or the strain for a fixed Ge concentration. Recent developments on the *V*-O, $V_2$, *V*-P, and *V*-Sb centers have been reported in $Si_{1-x}Ge_x$ alloys.[10–14] Most of these studies were done either on fully strained ($\tau=0$) or fully relaxed ($\tau=100\%$) $Si_{1-x}Ge_x$, where $\tau$ is the degree of strain relaxation. In a recent deep-level transient spectroscopy (DLTS) study,[10] a defect labeled E1 is observed in phosphorous (P-)doped fully strained $Si_{1-x}Ge_x$ alloys grown by chemical vapor deposition (CVD) and was tentatively attributed to *V*-P pair. Moreover, the activation enthalpy ($E_H$) of the level labeled E1 with respect to the conduction band edge in fully strained $Si_{1-x}Ge_x$ was found to remain constant for Ge content larger than 4%, but being much higher than that of Si.[10] However, for antimony (Sb-)doped totally relaxed $Si_{1-x}Ge_x$ alloys grown by molecular beam epitaxy (MBE),[11] the activation enthalpy was found to increase linearly with increasing Ge content. The sharp increase of 0.1 eV in $E_H$ observed between *V*-Sb in totally relaxed $Si_{0.95}Ge_{0.05}$ and the defect E1 in fully strained $Si_{0.96}Ge_{0.04}$ cannot be explained by the effect of strain alone, and it is in conflict with the increase of the band gap with increasing degree of strain relaxation $\tau$. In our recent study,

 ©2008 The American Physical Society

the activation enthalpy (~0.44 eV) of *V*-P for He-ion irradiated P-doped fully strained $Si_{1-x}Ge_x$ grown by CVD was found, within the experimental error, to be the same for $x=0$ and 0.04.[13] The activation enthalpy of the defect $E_1$ (~0.518 eV) reported by Monakhov *et al.*[10] for fully strained $Si_{0.96}Ge_{0.04}$ is different from $E_H$ of *V*-Sb ($E_H=0.45$ eV) in totally relaxed $Si_{0.95}Ge_{0.05}$ (Ref. 11) and from the value reported in our DLTS study of *V*-P center in P-doped fully strained $Si_{0.96}Ge_{0.04}$ ($E_H=0.44$ eV). These controversial findings about the position of *E* center make the situation ambiguous as regards to the effect of the composition and the strain on the electronic properties of *E* center in $Si_{1-x}Ge_x$ epilayers.

In fact, fully strained and partially relaxed $Si_{1-x}Ge_x$ can have the same bad gap for different Ge contents. This is because identical strain in $Si_{1-x}Ge_x$ can be obtained for different Ge contents. On one hand, this gives the possibility to control the band gap independently of the Ge content. On the other hand, one can monitor the Ge content independently of the band gap of the $Si_{1-x}Ge_x$ alloys. To the best of our knowledge, no published data were reported for DLTS studies on the position of the acceptor levels of $V_2$ and *V*-P centers when the band gap is modified only by strain relaxation in $Si_{1-x}Ge_x$ for a given Ge content.

Besides, one can evaluate the effect of irradiation on the functioning of $Si_{1-x}Ge_x$ based devices which can provide a thorough understanding of the degradation of electronic devices due to process-induced defects. It is therefore imperative to study the strain and composition effects on the electronic properties of the vacancy-related defects in $Si_{1-x}Ge_x$ alloys.

In this paper, we report on the study of He-ion irradiation induced defects in phosphorus-doped *n*-type Si, fully strained *n*-type $Si_{0.96}Ge_{0.04}$, and partially relaxed *n*-type $Si_{0.9}Ge_{0.1}$ epitaxially grown by CVD. On the basis of the composition and the strain effect on the activation enthalpy of the *V*-P pair in $Si_{1-x}Ge_x$, we show that the energy level of *E* center is independent of either the strain or the Ge content. In addition, we also show that the activation enthalpy of the second charge state of the divacancy $V_2^{=/-}$ decreases with increasing strain. Finally, the effect of the random distribution of Si and Ge atoms surrounding the *E* center on the related energy level is also addressed.

## II. EXPERIMENT

For this study, we have used epitaxial *n*-type (001) oriented Si and $Si_{0.9}Ge_{0.1}$ layers, grown by CVD on a lightly doped $[(4-6)\times10^{16}\ cm^{-3}]$ Si buffer layer which was grown on a $n^+$-Si substrate. The free carrier concentration induced by phosphorous doped material as determined by capacitance-voltage (*C-V*) measurements was $(8-6)\times10^{16}\ cm^{-3}$. The lattice parameters and degree of the strain in the $Si_{1-x}Ge_x$ films were deduced from high-resolution x-ray diffraction (HRXRD) measurements. From HRXRD measurements, it was confirmed that there was a lattice relaxation in the *n*-$Si_{0.9}Ge_{0.1}$ epilayers and the average relaxation factor was determined to be $\tau\approx22\%$.[15] The thickness of the $Si_{0.9}Ge_{0.1}$ epilayer was 480 nm which is well above

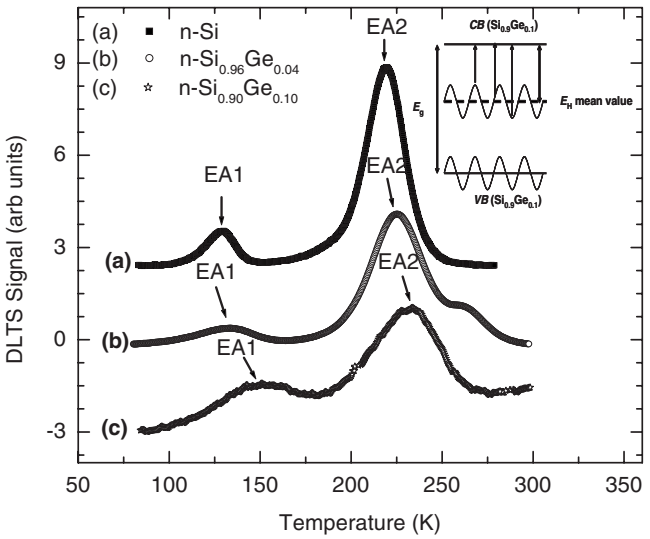


FIG. 1. Typical DLTS spectra obtained after (a) He-ion irradiated phosphorous-doped *n*-Si (b) fully strained *n*-$Si_{0.96}Ge_{0.04}$/Si, and (c) partially relaxed *n*-$Si_{0.9}Ge_{0.1}$/Si. The spectra were recorded at a lock-in amplifier frequency of 46 Hz using a filling pulse width of $t_p=0.2$ ms, a reverse quiescent bias of $V_r=0.5$ V, and a filling pulse amplitude of $V_p=0.8$ V. The inset is a schematic diagram of the corresponding transitions showing the distribution of the valence band induced by a fluctuation of the Ge content as well as the fluctuating emission rate ($e_n$) induced by nonhomogenous atomic environment surrounding the *V*-P pair.

the experimentally[16] and theoretically[17,18] calculated critical layer thickness. The Ge content ($x=0.04$ and 0.10) was determined by Rutherford backscattering spectrometry and was found to be uniform within the SiGe epilayers. After chemical cleaning, the circular palladium (Pd) Schottky contacts, 0.77 mm in diameter and 200 nm thick, were resistively evaporated on the *n*-type Si and $Si_{1-x}Ge_x$ through a metal contact mask. Schottky barrier diodes fabricated on clean Si and $Si_{1-x}Ge_x$ layers were irradiated with 5.4 MeV He ions from an $^{241}Am$ source to the fluence of $8\times10^{11}\ cm^{-2}$ at a dose rate of $7.1\times10^6\ cm^{-2}\ s^{-1}$.[13] For comparison purpose, control diodes on unimplanted $Si_{1-x}Ge_x$ samples were fabricated under identical experimental conditions.

In this investigation, our previous DLTS results on fully strained *n*-$Si_{0.96}Ge_{0.04}$ film were included in order to cover different Ge content values with different degrees of strain. The *n*-$Si_{0.96}Ge_{0.04}$ sample is grown by CVD, with the same doping concentration and under the same growth temperature as that for Si and $Si_{0.9}Ge_{0.1}$ samples. The details of the growth, fabrication, and characterization can be found in Ref. 13.

## III. RESULTS AND DISCUSSION

### A. Defects identification

Typical DLTS spectra from high energy He-ion irradiated *n*-type Si, fully strained $Si_{0.96}Ge_{0.04}$, and partially relaxed $Si_{0.90}Ge_{0.1}$ samples are shown in Fig. 1. The absence of peaks between 40 and 300 K in the DLTS spectrum of the control

TABLE I. DLTS signatures of defects introduced during 5.4 MeV He-ion irradiation of $n$-type Si and partially relaxed $n$-type $Si_{0.9}Ge_{0.1}/Si$.

| Defect label | Ge content | $E_H$ (eV) | $\sigma_{na}$ ($cm^2$) | $T_{peak}$[a] (K) | $E_T$ (eV) | Defect type |
|---|---|---|---|---|---|---|
| EA1 | 0 | 0.24 | $2.3\times10^{-16}$ | 129 | | $V-V^{=/-}$ |
| EA2 | 0 | 0.44 | $7.6\times10^{-16}$ | 220 | 0.438 | $V$-P |
| EA1 | 0.10 | 0.23 | $1.0\times10^{-15}$ | 150 | | $V-V^{=/-}$ |
| EA2 | 0.10 | 0.47 | $2.5\times10^{-15}$ | 232 | 0.445 | $V$-P |

[a]Peak temperature at a lock-in amplifier frequency of 46 Hz, i.e., a decay time constant of 9.23 ms.
[b]Energy level ($E_T$) determined at the corresponding temperature.

samples reflects the absence of defects in the epilayer, prior to He-ion irradiation. After irradiation, two peaks can be distinguished which can be labeled EA1 located in the range of 130–148 K and EA2 located at 220–232 K. Due to the low concentration of impurities in the CVD grown $n$-Si and $n$-$Si_{1-x}Ge_x$, ($x$=0.04 and 0.1), the observed defects in our Si, $Si_{0.96}Ge_{0.04}$, and $Si_{0.9}Ge_{0.1}$ samples are expected to be of intrinsic type. It is well known that the irradiation of either moderately or highly phosphorus-doped $n$-type Si leads usually to the introduction of pointlike defects such as the $E$ center ($V$-P pair), the two charge states of the divacancy, [($V_2^{=/-}$) and ($V_2^{-/0}$)], and the $V$-O center.[19,20] The latter level is not observed in our samples because of the low concentration of oxygen in our CVD epitaxial Si and $Si_{1-x}Ge_x$ ($x$ =0.04 and 0.1) samples. The $E$ center in Si, which gives rise to an acceptor level with an activation enthalpy of 0.44 eV below the conduction band ($E_c$), is known to overlap with the singly negative state of divacancy ($V_2^{-/0}$) located at 0.42 eV below $E_c$.[19,21] The doubly negative charge state of the divacancy ($V_2^{=/-}$) is reported to be located at 0.25 eV in high energy implanted $n$-type Si.[22] Since the $n$-Si and $n$-$Si_{1-x}Ge_x$ samples have been grown under identical conditions with similar doping concentrations, the defects introduced in $n$-Si are expected to be of the same type as those introduced in $n$-$Si_{1-x}Ge_x$ The electronic properties such as activation enthalpy ($E_H$) and apparent capture cross section ($\sigma_{na}$) values of these defects, as determined from Arrhenius plots, are given in Table I. Based on the above agreements, the most prominent peaks EA1 and EA2 (Fig. 1) are due to the $V_2^{=/-}$ and the superposition of both the $V_2^{-/0}$ and $V$-P pairs, respectively. In high energy particle irradiated $n$-Si, the ratio between the DLTS peaks of the ($V_2^{-/0}$) and ($V_2^{=/-}$) is expected to be close to 1:1.[21] Our results show that the ratios of the relative peak heights of the EA2 to those of EA1 are at least 1:0.2, 1:0.1, and 1:0.4 for Si, $Si_{0.96}Ge_{0.04}$, and $Si_{0.9}Ge_{0.1}$, respectively. Therefore, the main contribution to the peaks at 220 K in $n$-Si, at 225 K in fully strained $n$-$Si_{0.96}Ge_{0.04}$ and at 232 K in partially relaxed $n$-$Si_{0.9}Ge_{0.1}$, should be attributed to the $E$ centers. Furthermore, it is clear from the spectra in Fig. 1 that the peak positions of both defects EA1 and EA2 in $Si_{1-x}Ge_x$ shift toward high temperature with increasing Ge content. A similar trend was reported for the acceptor level $V$-Sb in $n$-$Si_{1-x}Ge_x$.[11] Moreover, a broadening and a decrease of the peak intensity of EA1 and EA2 are observed for both $n$-$Si_{0.96}Ge_{0.04}$ and $n$-$Si_{0.9}Ge_{0.1}$ relative to those observed for $n$-Si. We believe that this effect is due to the fluctuation of the atomic environment surrounding the defect levels, as will be discussed below. From now onward, the discussion will be limited to the defects EA1 and EA2 observed in partially relaxed $n$-$Si_{0.9}Ge_{0.1}$, since the same defects were observed in $n$-Si and fully strained $n$-$Si_{0.96}Ge_{0.04}$. Figure 2(a) depicts the DLTS spectra of He-ion irradiation induced defects in $n$-$Si_{0.9}Ge_{0.1}$ at different thermal-emission rates. In Fig. 2(b), we present the Arrhenius plot of $\ln(e_n/T^2)$ vs $1000/T$ of EA1 and EA2 in $n$-$Si_{0.9}Ge_{0.1}$ sample as deduced from the data of Fig. 2(a), where $e_n$ is the emission rate at temperature $T$. The values of $E_H$ and $\sigma_{na}$ of the He-ion irradiation induced defects EA1 and EA2 in $n$-$Si_{0.9}Ge_{0.1}$ sample were extracted from the slope and intercept of Arrhenius plot, respectively. The ($E_H$; $\sigma_{na}$) of EA1 and EA2 were determined for $n$-$Si_{0.9}Ge_{0.1}$ as (0.23 eV; $1.0\times10^{-15}cm^2$) and (0.47 eV; $2.5\times10^{-15}cm^2$), respectively. The experimental error is estimated to be ~10 meV using different repetition rates in the range from 2.2 to 220 Hz. For comparison purpose, Fig. 2(b) shows also the Arrhenius plot of the thermal-emission rate of $V$-P center (0.44 eV; $2.4\times10^{-15}$ $cm^2$) and the two charge states of divacancy, ($V_2^{-/0}$: 0.42 eV; $1.9\times10^{-16}$ $cm^2$) and ($V_2^{=/-}$: 0.25 eV; $1.3\times10^{-15}$ $cm^2$), as determined in irradiated $n$-type silicon.[19,22] As it is seen from this figure, the temperature dependence of thermal-emission rate corrected for $T^2(e_p/T^2)$ of defect EA2 lies between that of $V$-P pair and $V_2^{-/0}$ in $n$-type Si. In addition, the electron emission rate from the EA1 defect at given temperature is smaller than that observed for $V_2^{=/-}$ in $n$-Si. Thus, we identify level EA2 as that associated with the $V$-P center with a minor contribution from the singly charge state of the divacancy. This assignment is also supported by the fact that the phosphorous doping concentration in our $n$-Si and $n$-$Si_{0.9}Ge_{0.1}$ epilayers is relatively high ($\sim10^{17}$ $P/cm^{-3}$), and therefore the contribution of $V$-P center should be the most dominant in the irradiated sample. The extracted $E_H$ and $\sigma_{na}$ values of the level EA1 are in agreement with those observed for $V_2^{=/-}$ in $n$-Si (Ref. 22) and suggest that EA1 is associated with $V_2^{=/-}$.

The increase of the activation enthalpy of $V$-P pair in partially relaxed $Si_{0.90}Ge_{0.10}$ with respect to the value observed in Si is consistent with the observed linear behavior of the activation enthalpy for $V$-Sb with increasing Ge. On the other hand, the observed small decrease in the activation enthalpy of the double negative charge state of $V_2^{=/-}$ in partially relaxed $Si_{0.9}Ge_{0.1}$ with respect to Si is similar to that observed for single charge state of $V_2^{-/0}$ in fully strained $Si_{0.87}Ge_{0.13}$.[10] The compositional and strain dependences of

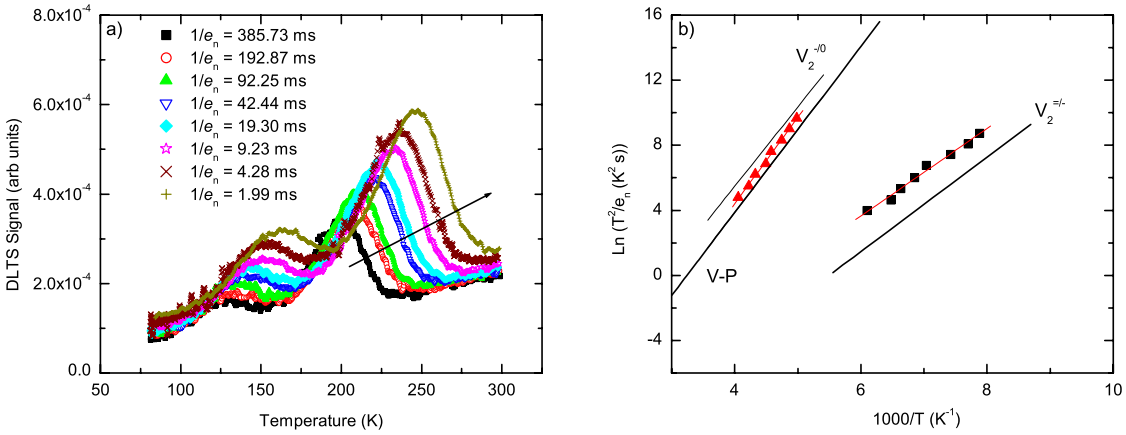


FIG. 2. (Color online) (a) DLTS spectra of He-ion irradiation induced defects in partially relaxed $n$-$Si_{0.9}Ge_{0.1}$/Si at different thermal-emission rate. All spectra were recorded using a filling pulse width of $t_p$=0.2 ms, a reverse quiescent bias of $V_r$=0.5 V, and a filling pulse amplitude of $V_p$=0.5 V. The arrow indicates the direction of decreasing the decay time constant (increasing thermal-emission rate $e_n$, respectively). (b) Arrhenius plots of the EA1 and EA2 peaks for partially relaxed $n$-$Si_{0.9}Ge_{0.1}$/Si. For comparison purposes, the solid lines represent the linear fit of the experimental data of the two charge state of the divacancy and the vacancy-phosphorous complex in pure $n$-Si (Ref. 19).

the activation enthalpy of both $V_2^{=/-}$ and $V$-P centers will be discussed in Secs. III B and III C, respectively.

### B. $V$-$V^{=/-}$ defect: Effect of composition and strain

Two factors can be at the origin of the change of $E_H$ of $V_2^{=/-}$: alloying and/or strain effects. Indeed, av Skardi *et al.*[23] have shown that $E_H$ of both $V_2^{=/-}$ and $V_2^{/0}$ in MBE grown fully relaxed $Si_{1-x}Ge_x$ increases with increasing Ge content. This increase in $E_H$ is most likely attributed to alloying effect only. Furthermore, Samara[24] using DLTS has demonstrated that the activation enthalpy of the $V$-P acceptor level relative to the conduction band increases with increasing hydrostatic pressure (29 meV/GPa), whereas that of the acceptor level $V_2^{=/-}$ of the divacancy decreases (−12 meV/GPa). The difference was explained in terms of lattice relaxation and its influence on the emission rate of electrons from these defects. For $V_2^{=/-}$, the lattice relaxes inward (outward) accompanying electron emission (electron capture). For $V$-P level, the lattice relaxes outward (inward) on electron emission (electron capture). At first glance, one may consider that the change of $E_H$ of $V_2^{=/-}$ in our $Si_{0.9}Ge_{0.1}$ sample with respect to Si is minute (relative change is about 10 meV). However, such relative change to the fully relaxed $Si_{0.9}Ge_{0.1}$ accounts for 45–50 meV. Therefore, the relative variation of $E_H$ in our samples with respect to fully relaxed SiGe at given Ge content can be reasonably attributed to strain effect. Due to the lattice mismatch between our $Si_{0.9}Ge_{0.1}$ and Si, a value of strain of about $3.3\times10^{-3}$ has been evaluated for the partially relaxed $Si_{0.9}Ge_{0.1}$ ($\tau$=20%) using Vegard's law. This value of strain is equivalent to 0.8 GPa using hydrostatic pressure. This would result in a shift of $E_H$ of maximum value of 10 meV. This is obviously smaller than the observed difference (45–50 meV) between $E_H$ in our $Si_{0.9}Ge_{0.1}$ sample and fully relaxed $Si_{0.9}Ge_{0.1}$. The large level shift in $E_H$ of $V_2^{=/-}$ between the fully relaxed SiGe and our partially relaxed SiGe samples for a given Ge content (10% Ge) can be explained by a relative inward large lattice relaxation accompanying electron emission from this defect upon strain. This is supported by the data from fully strained $Si_{0.96}Ge_{0.04}$.[13] The activation enthalpy of $V_2^{=/-}$ in fully strained is smaller as compared to fully relaxed SiGe with the same Ge content (4% Ge) (Ref. 23) and indicates again that the strain induces an inward lattice relaxation. The fully strained $Si_{0.96}Ge_{0.04}$ has a strain of about $1.7\times10^{-3}$ which is equivalent to hydrostatic pressure of 0.3 GPa and a strain shift in $E_H$ about 20 meV. Accordingly, in a coupling of 4% Ge and 10% Ge data, it seems that the strain reduces the activation enthalpy with strain coefficient of about 13.6 eV/u of strain which corresponds to 56 meV/GPa. This is also in agreement with recent reported results by Dobaczewski *et al.*,[25] where a stress-induced shift in the $V_2^{=/-}$ energy level in $n$-Si, ranging from 9 to 52 meV/GPa, depending on the crystallographic orientation, has been reported. Since our SiGe films exhibit biaxial strain, an average value in our case of 50–55 MeV/GPa is expected considering a combination of in-plane and out-of-plane strain effects.

### C. $V$-P defect: Effect of composition and strain

We focus on the $E$ center peaks in the temperature range of 200–250 K of Fig. 1. In order to study the effect of the Ge content and strain relaxation on the activation enthalpy of $V$-P, we have compared the DLTS "signatures" of this He-ion irradiation induced defect in fully strained $Si_{1-x}Ge_x$ ($x$ =0.04) and in partially relaxed ($x$=0.10) to those obtained in proton irradiation induced defects in fully strained[10] and fully relaxed $Si_{1-x}Ge_x$ (Ref. 11) with the same Ge content and compared this to the change in band gap with strain. The activation enthalpy of $V$-P center (EA2: 0.47 eV) in partially relaxed $Si_{0.9}Ge_{0.1}$ is close to the activation enthalpy of the $V$-Sb level (~0.47 eV) in fully relaxed $Si_{0.9}Ge_{0.1}$.[11] Similar comparison can also be made from fully strained $Si_{0.96}Ge_{0.04}$,[13] where the activation enthalpy of $V$-P pair

(EA2: 0.44 eV) is close to the previously reported $E_H$ (~0.45 eV) for *V*-Sb in antimony-doped totally relaxed $Si_{1-x}Ge_x$ films with $x=5\%$,[11] but differ from the value (0.51 eV) observed in phosphorous-doped fully strained $Si_{1-x}Ge_x$.[10]

The extracted apparent capture cross section of *V*-P is found to increase by a factor of 3 with increasing Ge content from 0% to 10% Ge. For $Si_{1-x}Ge_x$ ($x=0\%-10\%$), there is a systematic statistical uncertainties on $\sigma_{na}$ to be of the order of 10%, as estimated from the least-squares fit of the Arrhenius plots. Such trend of increasing apparent capture cross section with increasing Ge content has already been observed for the *V*-Sb pair in fully relaxed $Si_{0.9}Ge_{0.1}$.[11]

The thermal-emission rate $e_n$ of carriers from electron traps at temperature $T$ is expressed as[26]

$$e_n = \sigma_n \langle v_n \rangle N_C \exp\left[-\frac{E_T}{kT}\right]. \quad (1)$$

Here, $E_T$ is the energy of the defect below the conduction band minimum, $N_C$ is the effective density of states in the conduction band, $\langle v_n \rangle$ is the average thermal velocity of electrons, and $\sigma_n$ is the capture cross section. The physical parameter $E_T$ in Eq. (1) stands for Gibbs free energy and is given a priori by

$$E_T(x_{\mathrm{Ge}},T) = \Delta H(x_{\mathrm{Ge}},T) - T\Delta S(x_{\mathrm{Ge}},T), \quad (2)$$

where $x_{\mathrm{Ge}}$ is the Ge content, $T$ the temperature, and $\Delta H$ and $\Delta S$ are the respective changes in enthalpy and entropy due to the change in charge state of the level. When combining Eqs. (1) and (2), it follows that

$$e_n = \sigma_n \langle v_n \rangle N_C \exp\left[\frac{\Delta S}{k}\right]\exp\left[-\frac{\Delta H}{kT}\right]. \quad (3)$$

Therefore, the slope of an Arrhenius plot yields the enthalpy of the deep level $E_H=\Delta H$ (not the free energy) and $\sigma_{na}$ (intercept at $T^{-1}=0$) as determined from the Arrhenius plot, which is an *apparent* capture cross section, in which case the capture cross section $\sigma_n$ has the form

$$\sigma_n = \sigma_{na} \exp\left[-\frac{\Delta S}{k}\right]. \quad (4)$$

The extracted values of the apparent capture cross section of the *V*-P pair in Si and in partially relaxed $Si_{0.90}Ge_{0.10}$ fairly agree with the values previously reported for the *V*-Sb pair in Si and in fully relaxed $Si_{0.9}Ge_{0.1}$.[11] According to previous work,[11] the capture cross section of *E* center has been experimentally determined in fully relaxed $Si_{1-x}Ge_x$ to be $(6-8)\times 10^{-16}$ cm$^{-2}$ irrespective of the alloy composition. This value has been considered in the calculation of $\Delta S$ using Eq. (4). Based on Eq. (2), the energy level $E_T$ below the conduction band for *V*-P was then determined for *n*-Si and partially relaxed *n*-$Si_{0.9}Ge_{0.1}$ at the corresponding peak temperatures of 220 and 232 K, respectively. We found $0.44\pm0.01$ and $0.45\pm0.01$ eV for *V*-P in Si and in partially relaxed $Si_{0.9}Ge_{0.1}$, respectively. The results are summarized in Table I. The position of the energy level of the E center (*V*-P) in Si, in fully strained $Si_{096}Ge_{0.04}$ and in partially relaxed $Si_{0.9}Ge_{0.1}$ films, lies close to that reported for the *V*-Sb center in fully relaxed $Si_{1-x}Ge_x$. This implies that the energy depth of the *E*-center level from the conduction band does not depend either on Ge content or strain relaxation and indicates that such defect is pinned with respect to the conduction band.

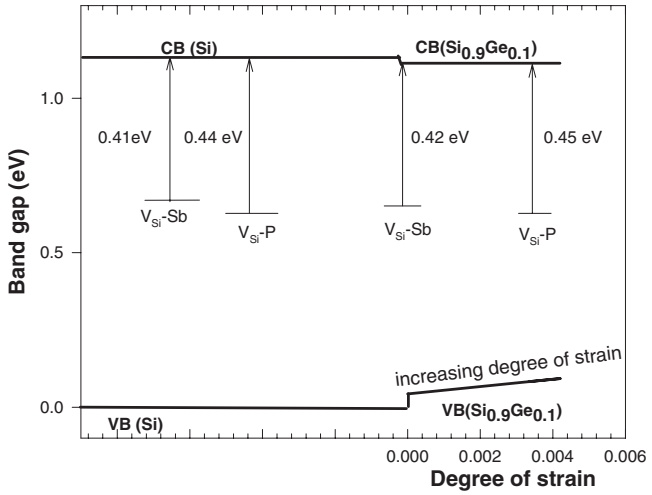


FIG. 3. Schematic representation illustrating the variation of the valence band and conduction band of $Si_{0.9}Ge_{0.1}$ with respect to that of Si as well as the *E* center energy level as a function of degree of strain. For clarity, the horizontal scale is applied only for $Si_{0.9}Ge_{0.1}$.

An interesting point to note is that the lattice constant of $Si_{0.9}Ge_{0.1}$ is 0.42% larger than that of Si. Hence, the fully strained $Si_{0.9}Ge_{0.1}$ has a strain of 0.42%. However, if the $Si_{1-x}Ge_x$ is biaxially compressed, the band gap of $Si_{1-x}Ge_x$ would be reduced by ~133 meV/% of biaxial compressive strain. Our partially relaxed $Si_{0.9}Ge_{0.1}$ ($\tau\approx 22\%$) has a remaining strain of 0.33% and its band gap is about 45 meV below that of fully relaxed $Si_{0.9}Ge_{0.1}$. Based on previous results showing that the band gap shrinkage results in an upward shift of the valence band,[27,28] also taking into account that the valence band offset is for at least 90% of the band gap difference between Si and strained $Si_{1-x}Ge_x$ as well as between the strained $Si_{1-x}Ge_x$ and the relaxed $Si_{1-x}Ge_x$ for a given Ge content,[27] and finally, setting the valence band of Si equal to the energy reference, the resulting band gap variation diagram as a function of degree of strain in $Si_{0.9}Ge_{0.1}$ can be deduced and is shown in Fig. 3. As seen from this diagram, the band gap narrowing in $Si_{0.9}Ge_{0.1}$ with increasing the degree of strain is entirely reflected in the valence band shift. Also, as shown in Fig. 3, the energy levels, with respect to the conduction band, of *V*-P and *V*-Sb in partially and fully relaxed $Si_{0.9}Ge_{0.1}$, respectively, are the same as those in Si. In addition within the experimental uncertainty, there is a fair agreement between the *V*-Sb and *V*-P energy level positions in *n*-Si and *n*-$Si_{0.9}Ge_{0.1}$ with respect to the conduction band. Therefore, the mean value of the energy position of the *E* center in the band gap for a given temperature should not exhibit either composition or strain relaxation dependence. This result suggests, as the case of *V*-Sb pair, that the deep level of *V*-P is pinned with respect to the conduction band. In accordance with Van de Walle and Martin,[28] the strain relaxation independent *E*-center energy level on *n*-type $Si_{1-x}Ge_x$ suggests solely the movement of the valence

band of $Si_{1-x}Ge_x$/Si heterostructure upon strain relaxation, as expected.

### D. Compositional fluctuation and broadening of *V*-P center

In order to study the effect of the relative distribution of either P or Sb at the Ge site on the defect level of the *E* center, a theoretical analysis was carried out using the full-potential linearized augmented plane wave method as employed in the WIEN2K code, where various forms of $V_{xc}$ are available.[29,30] In the calculation presented here, we have used the generalized gradient approximations of Perdew-Burke-Ernzerhof. Diamond structure unit cells of eight atoms and a lattice constant of 5.43 Å are used to study the total energy of P- or Sb-doped Si alloyed with small fraction of Ge. Out of eight atoms in the unit cell, one atom is Ge and one atom is either P or Sb. The P and Sb atoms are located as nearest neighbors of Ge or as next nearest neighbors. The angular momentum of $l_{\max}=10$ and atomic sphere radius $R_{MT}=2.2$ a.u. were used. The linearized augmented plane wave with local orbital bases was used for all valence states. The wave functions in the interstitial region were expanded in plane waves with a cutting off $K_{\max}=7/R_{MT}$, where $R_{MT}$ defined above as the atomic sphere radius and $K_{\max}$ gives the magnitude of the largest *K* vector of the plane wave expansion, while the electron density was Fourier expanded up to $G_{\max}=14$. A mesh of 343 special *k* points was taken for the irreducible Brillouin zone wedge. We found that the total energy when P or Sb is next nearest neighbors of Ge is lower than that when P or Sb is nearest neighbors by 0.004 and 0.09 eV, respectively. This indicates that the location of P relative to Ge is far less important in comparison to that of Sb. Hence, Sb will always be located further away from Ge. However, the calculation of the total energy as a function of the location of donor atoms (P or Sb) shows a nonpreferential location of P relative to Ge (far or closer to Ge atoms). The distribution of Ge atoms surrounding the P is assumed to be purely statistical leading to a local Ge fluctuation or disorder in the vicinity of the *V*-P defect.

It is worth noting that the relative decrease of the peak intensity of *V*-P and $V_2^{=/-}$ pairs in our partially relaxed $n$-$Si_{0.9}Ge_{0.1}$ as well as their broadening have also been observed by Kringhøj and Larsen in fully relaxed *n*-type SiGe.[11] A similar feature was observed for Au donor related level in fully relaxed *p*-type SiGe,[31] exclusively for transitions related the valence band. This has been attributed to the fluctuation of the band gap energy due to a variation of the maximum of the valence band induced by local fluctuation in the Ge alloy composition. A plausible explanation of the observed broadening of the acceptor *V*-P peak in our partially relaxed $n$-$Si_{0.9}Ge_{0.1}$ is sketched in the inset of Fig. 1. We consider that the statistical fluctuation of the atomic arrangement surrounding the *V*-P center based on our calculation above may induce a fluctuation in the related ionization energy level around a mean value ($E_H$). Hence, a distribution of carrier emission rate associated with electron transitions between the *V*-P level and the conduction band is expected.[32] This would result in a fluctuation of the associated activation enthalpy and then in a broadening of the corresponding peak defect. Therefore, the experimental observation presented above is in agreement with our theoretical calculation predicting fluctuation of the Ge atoms neighboring the P, and a fluctuating of atomic environment of the *E* center is assumed. This implies a broadening of a peak defect emerging from electron transitions between the *V*-P level and the conduction band. This interesting aspect related to the impact of the *statistical distribution of Ge* atoms and consequently a *statistical fluctuation of strain* around the *V*-P center inducing a *fluctuation of the E center energy level* should set forward further investigation on the subject.

## IV. CONCLUSION

In conclusion, DLTS studies of He-ion irradiated phosphorous-doped *n*-type Si and partially relaxed $Si_{0.90}Ge_{0.10}$ epilayer have been performed. It has been found that He-ion irradiation induced the same defects $V_2^{=/-}$ and *V*-P center in *n*-Si and $n$-$Si_{0.90}Ge_{0.10}$. It has been found that the activation enthalpy of $V_2^{=/-}$ in $n$-$Si_{0.90}Ge_{0.10}$ decreases slightly with respect to Si, while a large decrease of $E_H$ is observed between the partially relaxed $n$-$Si_{0.90}Ge_{0.10}$ and fully relaxed $n$-$Si_{0.90}Ge_{0.10}$. This large difference is explained by a large inward lattice relaxation and is suggested to be due to a combination of in-plane and out-of-plane strain effects. On the other hand, this study shows that the energy level of *E* center in $Si_{1-x}Ge_x$ does not change either with Ge content or strain relaxation and indicates that the *V*-P level is pinned below the conduction band. These findings regarding the strain independent *E* center energy level are suggesting the movement of the valence band of strained $Si_{1-x}Ge_x$/relaxed $Si_{1-x}Ge_x$ heterostructure upon relaxation only. Moreover, the random distribution of Ge atoms around the *V*-P center due to the chemical disorder is found to induce a fluctuation of the ionization energy level of the *E* center.

*mamor@squ.edu.om

[1] T. P. Pearsall, Mater. Sci. Eng., B **9**, 225 (1991).
[2] J. Vanhellemont, M.-A. Trauwaert, J. Poortmans, M. Caymax, and P. Clauws, Appl. Phys. Lett. **62**, 309 (1993).
[3] H. Ohyama, K. Hayama, J. Vanhellemont, J. Poortmans, M. Caymax, Y. Takami, H. Sunaga, I. Nashiyama, and Y. Uwatoko, Appl. Phys. Lett. **69**, 2429 (1996).
[4] G. D. Watkins and J. W. Corbett, Phys. Rev. **134**, A1359 (1964).
[5] G. D. Watkins and J. W. Corbett, Phys. Rev. **121**, 1001 (1961).
[6] J. W. Corbett and G. D. Watkins, Phys. Rev. Lett. **7**, 314 (1961).
[7] E. L. Elkin and G. D. Watkins, Phys. Rev. **174**, 881 (1968).
[8] A. O. Evwaraye, J. Appl. Phys. **48**, 734 (1977).
[9] F. D. Auret, A. R. Peaker, V. P. Markevich, L. Dobaczewski, and R. M. Gwilliam, Physica B **376-377**, 73 (2006).

[10] E. V. Monakhov, A. Yu. Kuznetsov, and B. G. Svensson, Phys. Rev. B **63**, 245322 (2001); J. Appl. Phys. **87**, 4629 (2000).
[11] P. Kringhøj and A. N. Larsen, Phys. Rev. B **52**, 16333 (1995).
[12] V. P. Markevich, A. R. Peaker, L. I. Murin, J. Coutinho, V. J. B. Torres, R. Jones, S. O. Berg, P. R. Briddon, F. D. Auret, and N. V. Abrosimov, Physica B **340-342**, 790 (2003).
[13] M. Mamor, H. Ouacha, M. Willander, F. D. Auret, S. A. Goodman, A. Ouacha, and E. Sveinbjörnsson, Appl. Phys. Lett. **76**, 3750 (2000).
[14] J. J. Goubet, D. Stievenard, D. Mathiot, and M. Zazoui, Phys. Rev. B **46**, 10113 (1992). J. J. Goubet and D. Stievenard, Appl. Phys. Lett. **66**, 1409 (1995).
[15] M. Mamor, O. Nur, M. Karlsteen, M. Willander, and F. D. Auret, J. Appl. Phys. **86**, 6890 (1999).
[16] J. C. Bean, L. C. Feldman, A. T. Fiory, S. Nakahara, and I. K. Robinson, J. Vac. Sci. Technol. A **2**, 436 (1984).
[17] J. W. Matthews and A. E. Blakeslee, J. Cryst. Growth **27**, 322 (1974).
[18] D. C. Houghton, J. Appl. Phys. **70**, 2136 (1991).
[19] S. D. Brotherton and P. Bradley, J. Appl. Phys. **53**, 5720 (1982).
[20] J. R. Troxell, Solid-State Electron. **26**, 539 (1983).
[21] B. G. Svensson and M. Willander, J. Appl. Phys. **62**, 2758 (1987).
[22] F. D. Auret, P. N. K. Deenapanray, S. G. Goodman, W. E. Meyer, and G. Myburg, J. Appl. Phys. **83**, 5576 (1998).
[23] H. av Skardi, A. Bro Hansen, A. Mesli, and A. Nylandsted Larsen, Nucl. Instrum. Methods Phys. Res. B **186**, 195 (2002).
[24] G. A. Samara, Phys. Rev. B **39**, 12764 (1989).
[25] L. Dobaczewski, K. Gościński, Z. R. Zytkiewicz, K. Bonde Nielsen, L. Rubaldo, O. Andersen, and A. R. Peaker, Phys. Rev. B **65**, 113203 (2002).
[26] G. L. Miller, D. V. Lang, and L. C. Kimerling, Annu. Rev. Mater. Sci. **7**, 377 (1977).
[27] D. C. Houghton, G. C. Aers, S. R. Eric Yang, E. Wang, and N. L. Rowell, Phys. Rev. Lett. **75**, 866 (1995).
[28] C. G. Van de Walle and R. M. Martin, Phys. Rev. B **34**, 5621 (1986).
[29] P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, and J. Luitz, WIEN2K, An Augmented Plane Wave+Local Orbitals Program for Calculating Crystal Properties, Karlheinz Schwarz, Technische Universitat Wien, Austria, 2001.
[30] S. Cottenier, *Density Functional Theory and the Family of (L)APW-Methods: A Step-by-Step Introduction* (Institute voor Kern-en Stralingsfysica, K. U. Leuven, Belgium, 2002).
[31] A. Mesli, P. Kringhøj, and A. N. Larsen, Phys. Rev. B **56**, 13202 (1997).
[32] A. Mesli, V. I. Kolkovsky, L. Dobaczewski, A. Nylandsted Larsen, and N. V. Abrosimov, Nucl. Instrum. Methods Phys. Res. B **253**, 154 (2006).