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# Vacancy-oxygen defects in $p$ -type $\text{Si}_{1-x}\text{Ge}_x$

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## Abstract

Oxygen-vacancy defects and in particular the VO pairs (known as A-centers) are common defects in silicon (Si) with a deleterious impact upon its properties. Although oxygen-vacancy defects have been extensively studied in Si there is far less information about their properties in  $p$ -type doped silicon germanium ( $\text{Si}_{1-x}\text{Ge}_x$ ). Here we use Fourier transform infrared spectroscopy (FTIR) to determine the production and evolution of oxygen-vacancy defects in  $p$ -type  $\text{Si}_{1-x}\text{Ge}_x$ . It was determined that the increase of Ge content affects the production and the annealing behavior of the VO defect as well as its conversion to the  $\text{VO}_2$  defect. In particular both the VO production and the VO annealing temperature are reduced with the increase of Ge. The conversion ratio  $[\text{VO}_2]/[\text{VO}]$  also decreases with the increase of  $x$ , although the ratios  $[\text{VO}_3]/[\text{VO}_2]$  and  $[\text{VO}_4]/[\text{VO}_3]$  show a tendency to increase for larger Ge contents. The results are discussed in view of recent experimental and theoretical studies in Si and  $\text{Si}_{1-x}\text{Ge}_x$ .

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## I. INTRODUCTION

In the past few years the requirement to substitute Si with higher carrier mobility substrates has led to the consideration of  $\text{Si}_{1-x}\text{Ge}_x$  and germanium (Ge).<sup>1-5</sup> An enabling factor is the advent of high dielectric constant (high- $k$ ) dielectrics that allow the departure from the prerequisite to use native oxides such as  $\text{SiO}_2$  in Si-based devices.<sup>6-8</sup>  $\text{Si}_{1-x}\text{Ge}_x$  is a random alloy with the diamond structure that has one lattice site that can be occupied by either Si or Ge. The variation of its properties (such as band gap, electron and hole mobility, and lattice parameter) with respect to the Ge content is particularly important for microelectronic and optoelectronic devices.<sup>9,10</sup> Interestingly, in previous experimental and theoretical studies it was shown that the structure and defect processes do not exhibit a Vegard law type behavior.<sup>11,12</sup> That is they cannot be determined by a simple linear interpolation of the respective properties of Si and Ge, which are the end members of  $\text{Si}_{1-x}\text{Ge}_x$ . The deviations are typically larger for intermediate Ge contents, however, they can appear to be non-existent for very small or very large Ge contents. Importantly, vacancies in  $\text{Si}_{1-x}\text{Ge}_x$  preferentially reside near at least one Ge atom as was determined by the positron annihilation spectroscopy (PAS) study of Sihto *et al.*<sup>13</sup> This has also been supported by recent density functional theory (DFT) studies.<sup>11,14</sup>

The defect processes of oxygen-related defects in  $\text{Si}_{1-x}\text{Ge}_x$  alloys are not understood or studied to the level they are in Si.<sup>15-17</sup> The A-center is composed of a  $V$  and an O interstitial ( $\text{O}_i$ ) atom therefore the energetics of its formation will be the balance of these two constituent point defects. Previous investigations have revealed that  $\text{O}_i$  preferentially bonds with two Si atoms (and is repelled from Ge atoms), whereas  $V$  are attracted to Ge atoms.<sup>18-20</sup> In  $\text{Si}_{1-x}\text{Ge}_x$  the Ge content has an impact upon the diffusion of

oxygen as well as the conversion of the VO to VO<sub>2</sub> clusters.<sup>21-23</sup> The aim of the present contribution is to study, using FTIR, the importance of Ge content on the production, evolution, and annealing of oxygen-vacancy defects in *p*-type Si<sub>1-x</sub>Ge<sub>x</sub> ( $x = 0.015, 0.028, 0.056$ ).

## II. EXPERIMENTAL METHODOLOGY

The samples were cut from Czochralski grown *p*-type Si<sub>1-x</sub>Ge<sub>x</sub> boron (B) doped wafers, acquired by the Institute of crystal growth in Berlin. The concentrations of B and Ge of the wafers were determined by the provider. The Ge concentration of the crystals varied from 1.5 – 5.6 %. B was introduced during growth at a concentration of 10<sup>15</sup> cm<sup>-3</sup>.<sup>24,25</sup> The oxygen and carbon concentrations of the samples were in the range of (5-11) 10<sup>17</sup> cm<sup>-3</sup> and (2-5) 10<sup>16</sup> cm<sup>-3</sup>, respectively. The samples were irradiated with 2MeV electrons at a temperature of 95 °C and a fluence of 5x10<sup>17</sup> cm<sup>-2</sup> at the Takasaki Jaeri Dynamitron Accelerator. Thereafter the samples were subjected to 20 min isochronal anneals from 50 to 550 °C with steps of 10 °C. Following every annealing step, the IR spectra were recorded at room temperature using an FTIR spectrometer.

## III. RESULTS

Figure 1 shows a characteristic segment of IR spectra of the *p*-type Si<sub>1-x</sub>Ge<sub>x</sub> ( $x = 0.015, 0.028, 0.056$ ) samples after irradiation and at selective temperatures (50 °C, 400 °C, 500 °C and 560 °C) in the course of the 20 min isochronal anneals sequence. Immediately after irradiation we can see the IR bands of the VO (830 cm<sup>-1</sup>) peak and at higher temperatures the VO<sub>2</sub> (888 cm<sup>-1</sup>), VO<sub>3</sub> (904, 967, 1000 cm<sup>-1</sup>), and VO<sub>4</sub> (985, 1010

$\text{cm}^{-1}$ ) peaks. Notably, for  $x = 0.056$  the signals of  $\text{VO}_4$  bands are very weak (refer to Fig. 1(c)). In the latter figure the bands of  $\text{C}_i\text{O}_i$  ( $862 \text{ cm}^{-1}$ ) and  $\text{C}_i\text{O}_i(\text{Si}_i)$  ( $1020 \text{ cm}^{-1}$ ) are present. These defects are not in the interest of the present study.

Figure 2 presents the thermal evolution of the  $\text{VO}$  ( $830 \text{ cm}^{-1}$ ), the  $\text{VO}_2$  ( $888 \text{ cm}^{-1}$ ), the  $\text{VO}_3$  ( $904, 967, 1000 \text{ cm}^{-1}$ ), and the  $\text{VO}_4$  ( $985, 1010 \text{ cm}^{-1}$ ) defects of the  $p$ -type  $\text{Si}_{1-x}\text{Ge}_x$  ( $x = 0.015, 0.028, 0.056$ ) samples. We note that in the  $x = 0.056$  sample the two bands of the  $\text{VO}_4$  defect are very weak and only the evolution of the  $985 \text{ cm}^{-1}$  band can be shown.

Figure 3 shows the thermal evolution of the  $\text{VO}$  ( $830 \text{ cm}^{-1}$ ) and the  $\text{VO}_2$  ( $888 \text{ cm}^{-1}$ ) bands for the  $p$ -type  $\text{Si}_{1-x}\text{Ge}_x$  ( $x = 0.015, 0.028, 0.056$ ) samples in a collective manner for comparison purposes. It is observed that the  $\text{VO}$  amplitudes for the  $x = 0.028$  and  $0.056$  samples are almost equal but lower compared to  $x = 0.015$ . Additionally, the amplitudes of the  $\text{VO}_2$  bands are decreasing with increasing  $x$ . We also observe that the annealing of  $\text{VO}$  defect occurs at around  $180 \text{ }^\circ\text{C}$ .

By inspection of Fig. 1 it is observed the full-width half maximum (FWHM) of the  $\text{VO}$  band increases with the increasing  $x$ . This is an indication of additional contributions to the shape of the  $\text{VO}$  band and necessitates Lorentzian profiling to investigate the contributing structures. Figure 4 depicts the Lorentzian deconvolution of the frequency range of the A-center band in the spectra for the  $x = 0.028$  and  $0.056$  samples, respectively. Regarding the  $x = 0.056$  sample (refer to Fig. 4(b)), besides the  $\text{VO}$  band at  $829 \text{ cm}^{-1}$ , two bands at  $834$  and  $841 \text{ cm}^{-1}$  could be detected indicating the presence of additional structures in the frequency range around the  $\text{VO}$  band. However, in the case of the  $x = 0.028$  sample (refer to Fig. 4(a)) only one band at  $834 \text{ cm}^{-1}$  is initially

observed. The  $841\text{ cm}^{-1}$  band is also observed but at higher temperatures (above  $220\text{ }^{\circ}\text{C}$ ). Additionally, a band at  $822\text{ cm}^{-1}$  is present in both samples.

Figure 5 shows the evolution of the  $829$ ,  $834$  and  $841\text{ cm}^{-1}$  bands for the  $x = 0.028$  and  $0.056$ . The VO band begins to decay around  $180\text{ }^{\circ}\text{C}$  accompanied initially by the enhancement of the  $834$  and  $841\text{ cm}^{-1}$  bands. Finally, as the annealing temperature increases further, all the contributing bands decay around  $250\text{ }^{\circ}\text{C}$  disappearing from the spectra at  $\sim 350\text{ }^{\circ}\text{C}$ . Simultaneously with their decay another band at  $888\text{ cm}^{-1}$  attributed to the  $\text{VO}_2$  defect emerges.

Figure 6 shows the  $a_{\text{VO}}$  with respect to the Ge concentration as derived from the Lorentzian profiles. Clearly, the VO amplitude decreases when the  $x$  increases.

A thorough inspection of the received spectra revealed that the shape of the  $888\text{ cm}^{-1}$  band is disturbed, a clear indication of the existence of additional components. Apparently, these bands originate from alternative structures which give rise to IR signals in the same spectral range. Figure 7 shows the Lorentzian deconvolution of  $\text{VO}_2$  band. At least two additional components at  $892$  and  $896\text{ cm}^{-1}$  seem to contribute in the shape of the spectral range of the  $\text{VO}_2$  defect.

Figure 8 represents the dependence of the ratio of the absorption coefficients of  $\text{VO}_{n+1}$  over  $\text{VO}_n$  with respect to the Ge concentration for the  $p$ -type  $\text{Si}_{1-x}\text{Ge}_x$  samples. It is observed that the  $a_{\text{VO}_2}/a_{\text{VO}}$  decreases with the increase of  $x$ , whereas the  $a_{\text{VO}_3}/a_{\text{VO}_2}$  and  $a_{\text{VO}_4}/a_{\text{VO}_3}$  ratios show the opposite trend.

#### IV. DISCUSSION

Lindström and Svensson<sup>15</sup> have established that a large percentage of A-centers in Si are transformed into  $VO_2$  clusters. However, in  $n$ -type  $Si_{1-x}Ge_x$  this fraction decreases<sup>23</sup> as the Ge-content increases. This is observed also here for the  $p$ -type  $Si_{1-x}Ge_x$ . It has been reported<sup>17,26</sup> that with the increase of the Ge content of the  $Si_{1-x}Ge_x$  material the amplitude of the VO band decreases although the FWHM of the band increases. The increase of FWHM has been attributed to additional contributions to the shape of the VO band originating from (VO-Ge) structures with the Ge atoms in adjacent positions to a VO core. In particular, Lorentzian profiling<sup>17,23,26</sup> of the band has attributed two bands at  $\sim 834$  and  $839\text{ cm}^{-1}$  to a  $(VO-Ge)_1$  and  $(VO-Ge)_2$  structures with the Ge atom in the first and second neighbour position in relation with VO, correspondingly. On the other hand, a reduction in the amplitude of the VO band was also verified<sup>21,22,27</sup> by deep level transient spectroscopy (DLTS) and Laplace DLTS spectroscopy studies. In our case of  $p$ -type  $Si_{1-x}Ge_x$  material the deconvolution procedure has shown (refer to Fig. 4) that besides the above two bands at  $834$  and  $841\text{ cm}^{-1}$ , another band at  $822\text{ cm}^{-1}$  is also present. The latter band may be correlated with the  $V_2O_2$  defect.<sup>28</sup>

The observed decrease of VO concentration (refer to Fig. 6) was attributed<sup>17,26</sup> to the ability of Ge atoms to act as annihilation centers for primary defects, that is vacancies and self-interstitials (I), thus reducing the availability of vacancies to be trapped by oxygen atoms. In other words, it was suggested that as a result of the Ge presence, the annihilation rate of the components of Frenkel pairs produced by irradiation was increased, resulting in a decrease in the production of oxygen-vacancy pairs.

For both  $n$ - and  $p$ -type  $\text{Si}_{1-x}\text{Ge}_x$  the  $\text{VO}$  pair is stable up to  $\sim 180$  °C, whereas in  $n$ - and  $p$ -type Si it is stable up to about  $\sim 250$  °C (refer to Fig. 2 and to Ref. 23 for  $n$ -type  $\text{Si}_{1-x}\text{Ge}_x$ ). The common behavior exhibited suggests that the lowering of the annealing temperature of the  $\text{VO}$  pair can be attributed to the host materials and not the  $p$ -type doping. It has been previously established by Kube *et al.*<sup>12</sup> (and references therein) that the increase of the Ge concentration of the  $\text{Si}_{1-x}\text{Ge}_x$  alloys leads to the lowering of the activation enthalpy of diffusion of dopants migrating via vacancy-related mechanisms. In essence, the introduction of the Ge leads to the formation of Si-Ge and Ge-Ge bonds (the latter is more populous at high Ge concentrations) that are weaker compared to the Si-Si bonds. Also the Si-Si bond lengths in  $\text{Si}_{1-x}\text{Ge}_x$  are increased due to the presence of the Ge atoms. These effects lower the annealing temperature of the  $\text{VO}$  pairs in  $\text{Si}_{1-x}\text{Ge}_x$  as compared to Si. An additional argumentation on the lowering of the annealing temperature based on the reactions that participate in the annealing of  $\text{VO}$  is presented below.

The observed decrease in the  $\text{VO}_2$  formation (refer to Fig. 3) as the Ge content of the  $\text{Si}_{1-x}\text{Ge}_x$  material increases could be attributed to the following scenario:

(i) Due to the formation of  $(\text{VO-Ge})$  structures less  $\text{VO}$  are available<sup>26</sup> to be transformed in  $\text{VO}_2$  centers and this is manifested in the spectra by the reduction of the  $888\text{ cm}^{-1}$  band amplitude in the spectra.

(ii) The annealing of  $\text{VO}$  defects is mainly governed by two reactions:  $\text{VO} + \text{O}_i \rightarrow \text{VO}_2$  and  $\text{VO} + \text{I} \rightarrow \text{O}_i$ . It has been suggested<sup>29</sup> that the strain fields induced in the  $\text{Si}_{1-x}\text{Ge}_x$  material due to the presence of the larger Ge atoms affect the availability of self-interstitials. In effect this changes the balance between the above two reactions and their



contribution in the VO annealing. Notably, for Ge-doped Si<sup>29</sup> it was argued that the larger the Ge content, the stronger and more extensive the strain fields in the material. As a result, the binding energy of self-interstitials in the large self-interstitial clusters<sup>30</sup> (which are the source of self-interstitials) is reduced leading to an increase of the number of available self-interstitials with the increase of Ge. Thus the contribution of the reaction  $VO + I \rightarrow O_i$  is enhanced and that of the reaction:  $VO + O_i \rightarrow VO_2$  is reduced. In essence, the whole process leads to a reduction of the  $VO_2$  formation as well as earlier lower annealing temperature of VO pairs due to the earlier activation of the  $VO + I \rightarrow O_i$  reaction. Indeed, in the  $Si_{1-x}Ge_x$  material VO signal begins to decay from the spectra at a lower temperature than in Si.

(iii) In another approach, one could consider the ability of Ge atoms to capture self-interstitials besides vacancies. In a previous report<sup>31</sup> regarding Ge-doped Si it was suggested that Ge atoms compete with C atoms in capturing self-interstitials. This competition becomes significant when  $[Ge]/[C]$  is larger than 1000. We extend this conclusion for  $Si_{1-x}Ge_x$  and in our case where the  $[Ge]/[C]$  ratio is much larger than three orders of magnitude this competition is stronger. As a result  $Ge_i$  form ( $Ge + Si_i \rightarrow Ge_i$ ), which being mobile are immediately trapped by oxygen atoms to form  $GeO_i$  pairs. Notably, the formation of such centers has been previously considered in the literature.<sup>32,33</sup> DFT results indicate that Ge repels  $O_i$ .<sup>32</sup> IR signals from such a center were not reported. This does not mean that the defect is not existent. Its signal may be very weak or the defect is IR inactive. These centers may dissociate above 200 °C producing  $Ge_i$  (via the reaction  $Ge_iO \rightarrow Ge_i + O_i$ ). Then the  $Ge_i$  atoms immediately convert to Ge atoms by releasing self-interstitials, which in turn react with VO centers

(VO + I  $\rightarrow$  O<sub>i</sub>). Thus less VO centers are available for the reaction VO + O<sub>i</sub>  $\rightarrow$  VO<sub>2</sub> and therefore less VO<sub>2</sub> centers are formed. The annealing of VO at a lower temperature is also explained in this scenario by the same reasoning as in scenario (ii).

As we succinctly mentioned in the results section the shape of the VO<sub>2</sub> band is disturbed and Lorentzian profiling has shown the existence of two additional contributed bands at 892 and 896 cm<sup>-1</sup>. These bands are similar to those observed in our previous work<sup>23</sup> in *n*-type Si<sub>1-x</sub>Ge<sub>x</sub>. They were attributed to (VO<sub>2</sub>-Ge)<sub>1</sub> and (VO<sub>2</sub>-Ge)<sub>2</sub> defects originating from structures with the Ge atoms in the first and the second neighbour position in relation with a VO<sub>2</sub> core.

Considering the formation of the VO<sub>3</sub> and VO<sub>4</sub> clusters, the species that needs to migrate is O<sub>i</sub> (note that in the case of VO<sub>2</sub> formation, VO is the migrating species) and it was previously determined that Ge enhances the O<sub>i</sub> diffusivity.<sup>34</sup> In addition, previous calculations<sup>35</sup> have deduced that the strain fields due to the larger Ge atoms lead to a reduction of the potential barrier height, thus enhancing the diffusion of oxygen. Therefore, the present results (refer to Fig. 8) are consistent as they represent an increase of the ratio of the absorption coefficients of VO<sub>n+1</sub> over VO<sub>n</sub> (n = 2, 3) that translates to a higher percentage of VO<sub>3</sub> and VO<sub>4</sub> clusters forming as the Ge content is increased.

#### IV. SUMMARY

In the present study we used FTIR spectroscopy to investigate the production and evolution of A-centers in *p*-type Si<sub>1-x</sub>Ge<sub>x</sub>. It was verified that the increase of Ge content results i) in the decrease of VO production, ii) in the decrease of VO annealing temperature and iii) in a decrease of the a<sub>VO<sub>2</sub></sub>/a<sub>VO</sub> ratio. Additionally, Lorentzian profiling

has detected bands related to (VO-Ge) structures as in the case of  $n$ -type  $\text{Si}_{1-x}\text{Ge}_x$ . Furthermore, the shape of the  $\text{VO}_2$  band was found to be disturbed by components related to the (VO<sub>2</sub>-Ge) structures. These issues will need to be systematically investigated from different perspectives (advanced computational modeling and further experiments over a wider range of Ge concentrations). The present study is part of a concerted effort to unravel the defect processes of group IV random alloys.

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## FIGURE CAPTIONS

**FIG. 1** Segments of the IR spectra of the *p*-type  $\text{Si}_{1-x}\text{Ge}_x$  ( $x = 0.015$  (a), 0.028 (b) and 0.056 (c)) samples after irradiation and at 50 °C, 400 °C, 500 °C and 560 °C in the course of the 20 min isochronal anneals sequence.

**FIG. 2** The thermal evolution of the VO (830  $\text{cm}^{-1}$ ), the  $\text{VO}_2$  (888  $\text{cm}^{-1}$ ), the  $\text{VO}_3$  (904, 967, 1000  $\text{cm}^{-1}$ ), and the  $\text{VO}_4$  (888, 1010  $\text{cm}^{-1}$ ) bands of the *p*-type  $\text{Si}_{1-x}\text{Ge}_x$  ( $x = 0.015$  (a), 0.028 (b) and 0.056 (c)) samples, in the course of the 20 min isochronal anneals sequence.

**FIG. 3** Comparison of the thermal evolution curves of the VO (830  $\text{cm}^{-1}$ ) and the  $\text{VO}_2$  (888  $\text{cm}^{-1}$ ) bands between the  $x = 0.015$ , 0.028 and 0.056 samples, in the course of the 20min isochronal anneal sequence.

**FIG. 4** Deconvolution of the A-center region IR bands into Lorentzian profiles at selected temperatures of the 20 min isochronal anneals sequence for the  $x = 0.028$  and 0.056 samples. Solid lines represent the experimental results; dotted lines the Lorentzian profiles and dashed lines the best fitting curves.

**Fig. 5** The evolution of the VO (829  $\text{cm}^{-1}$ ),  $(\text{VO-Ge})_1$  (841  $\text{cm}^{-1}$ ) and  $(\text{VO-Ge})_2$  (834  $\text{cm}^{-1}$ ) bands for the  $x = 0.028$  and 0.056 samples. The evolution of the 822  $\text{cm}^{-1}$  band is also shown.

**Fig. 6** The absorption coefficient of VO ( $a_{\text{VO}}$ ) with respect to the Ge concentration in *p*-type  $\text{Si}_{1-x}\text{Ge}_x$ .

**Fig. 7** Deconvolution of the  $\text{VO}_2$  region IR bands into Lorentzian profiles at a representative temperature of the 20 min isochronal anneals sequence for the  $x = 0.028$

sample. Solid lines represent the experimental results; dotted lines the Lorentzian profiles and dashed lines the best fitting curves.

**Fig. 8** The conversion ratio of the  $a_{VO2}/a_{VO}$ ,  $a_{VO3}/a_{VO2}$  and  $a_{VO4}/a_{VO3}$  with respect to the Ge concentration.



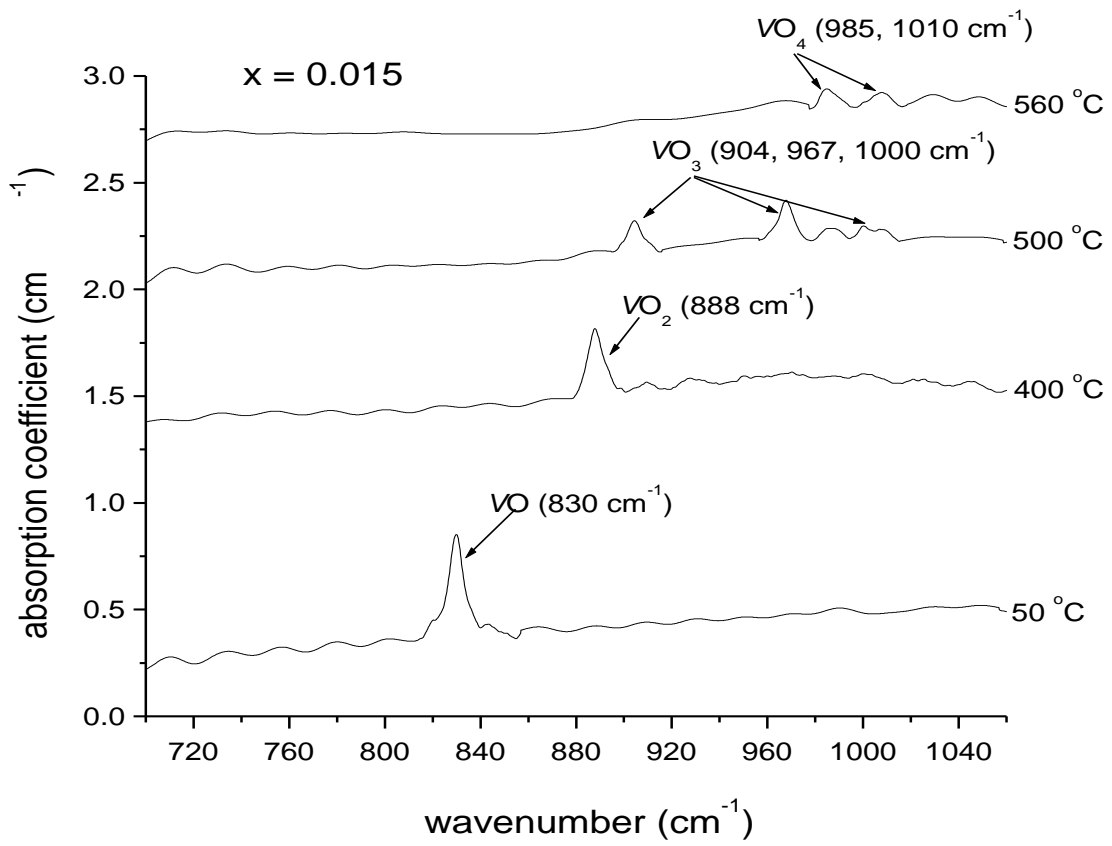


Fig. 1(a)

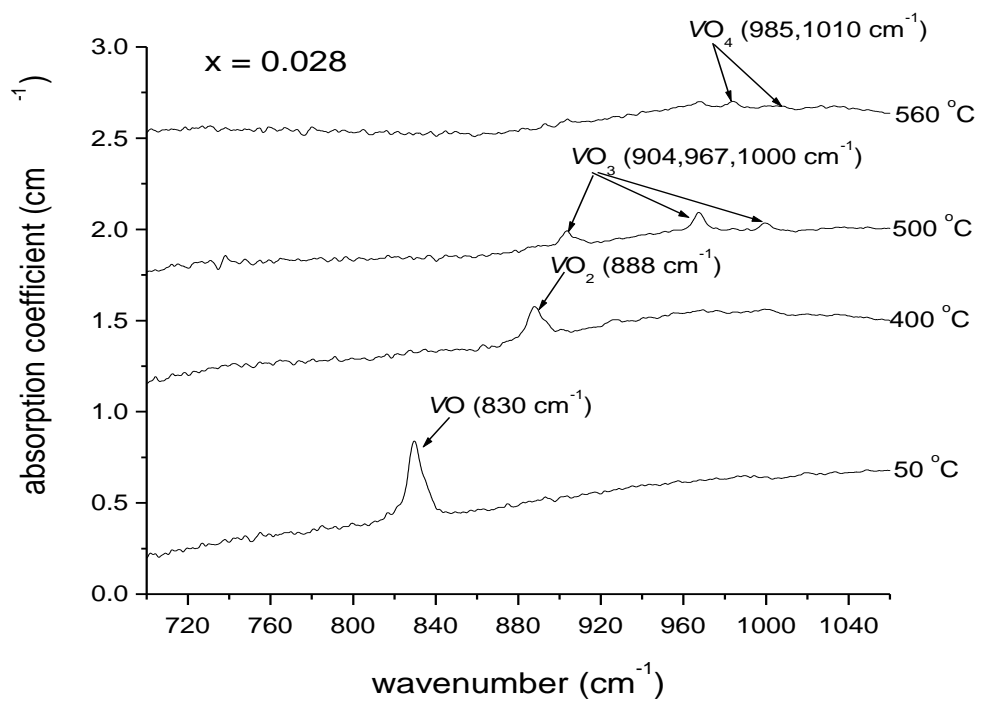


Fig. 1(b)

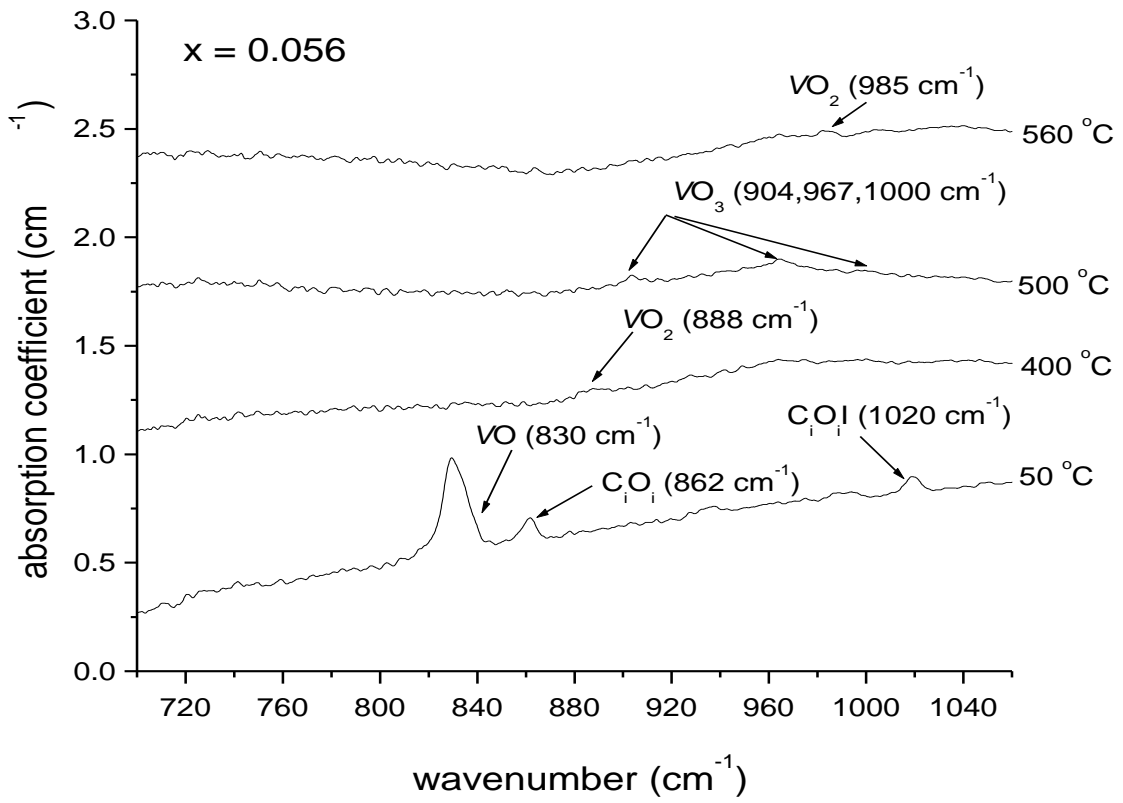


Fig. 1(c)

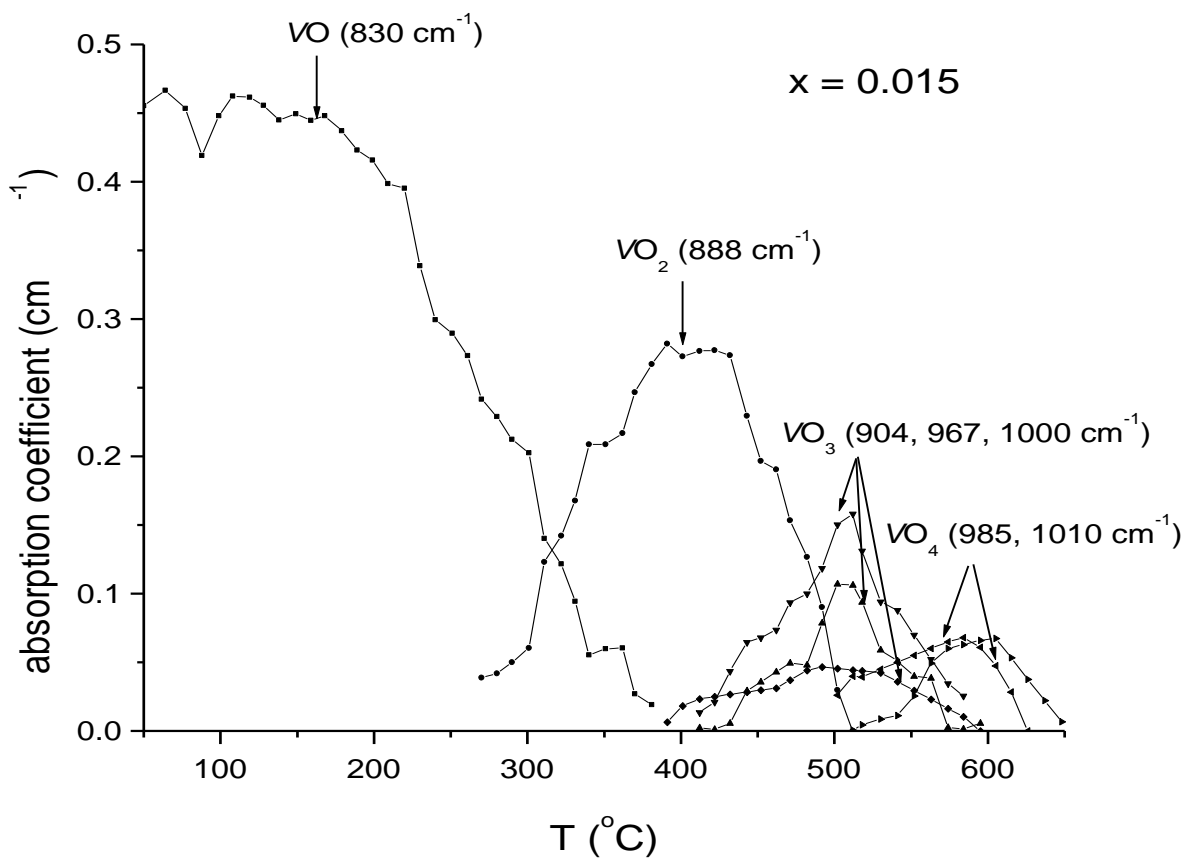


Fig. 2(a)

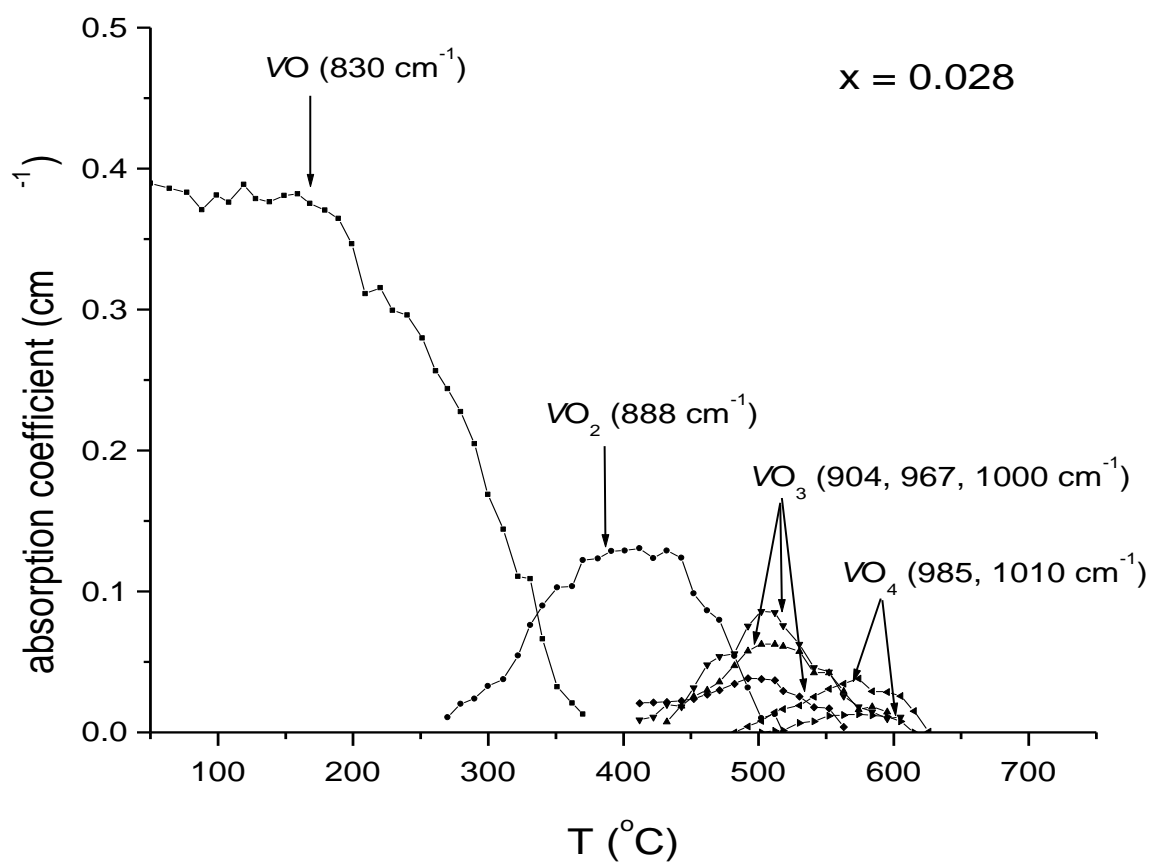


Fig. 2(b)

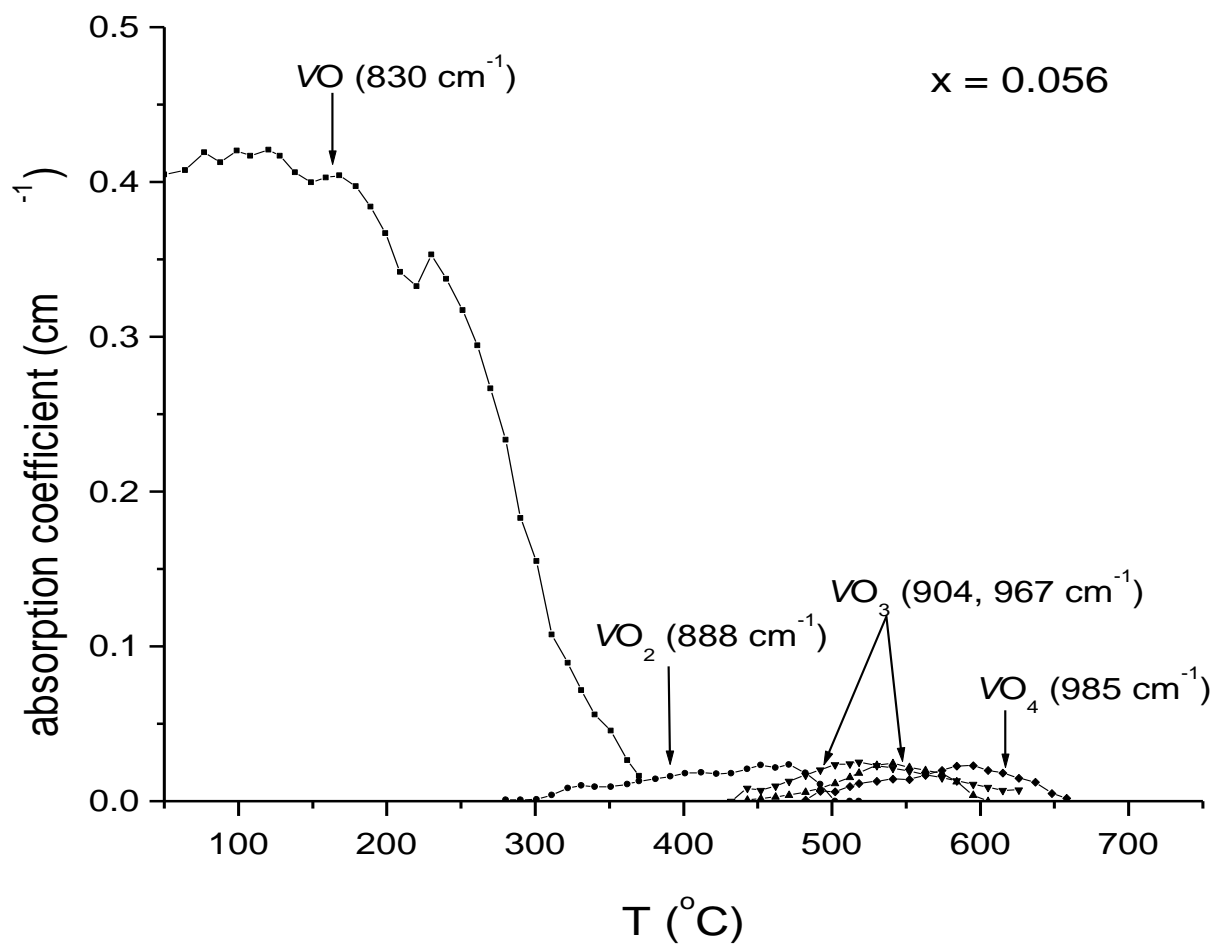


Fig. 2(c)

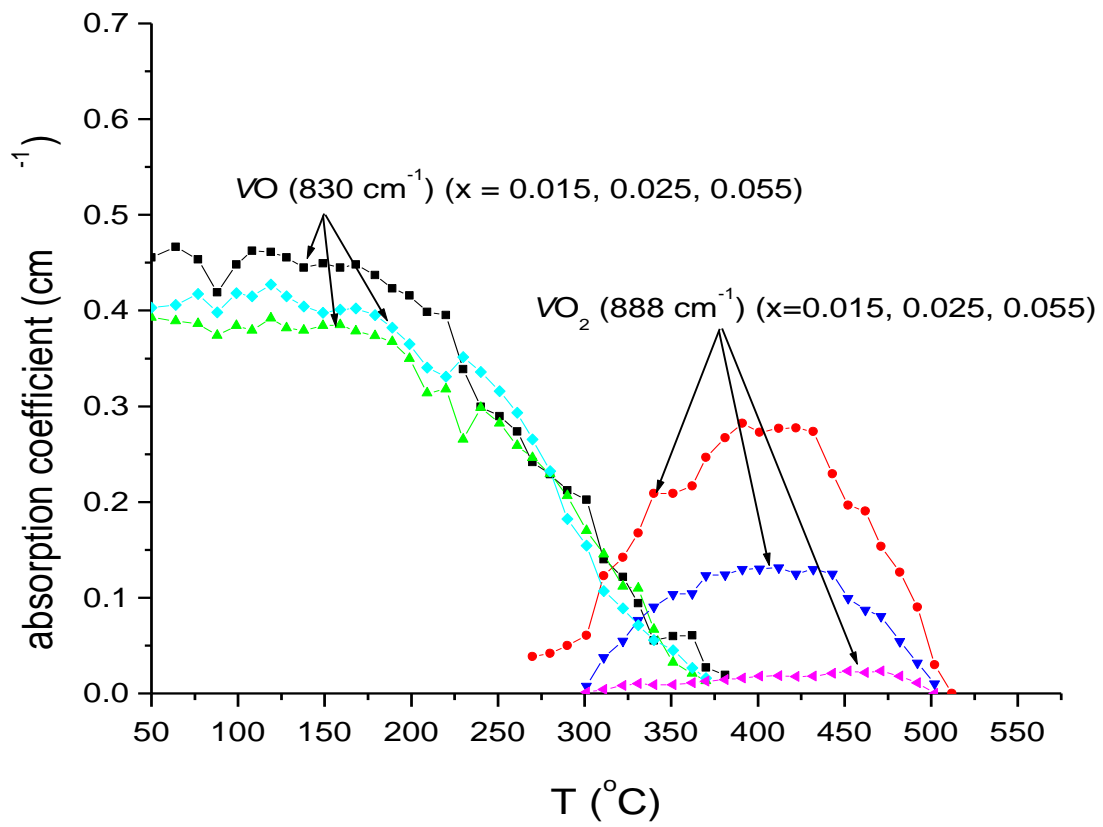
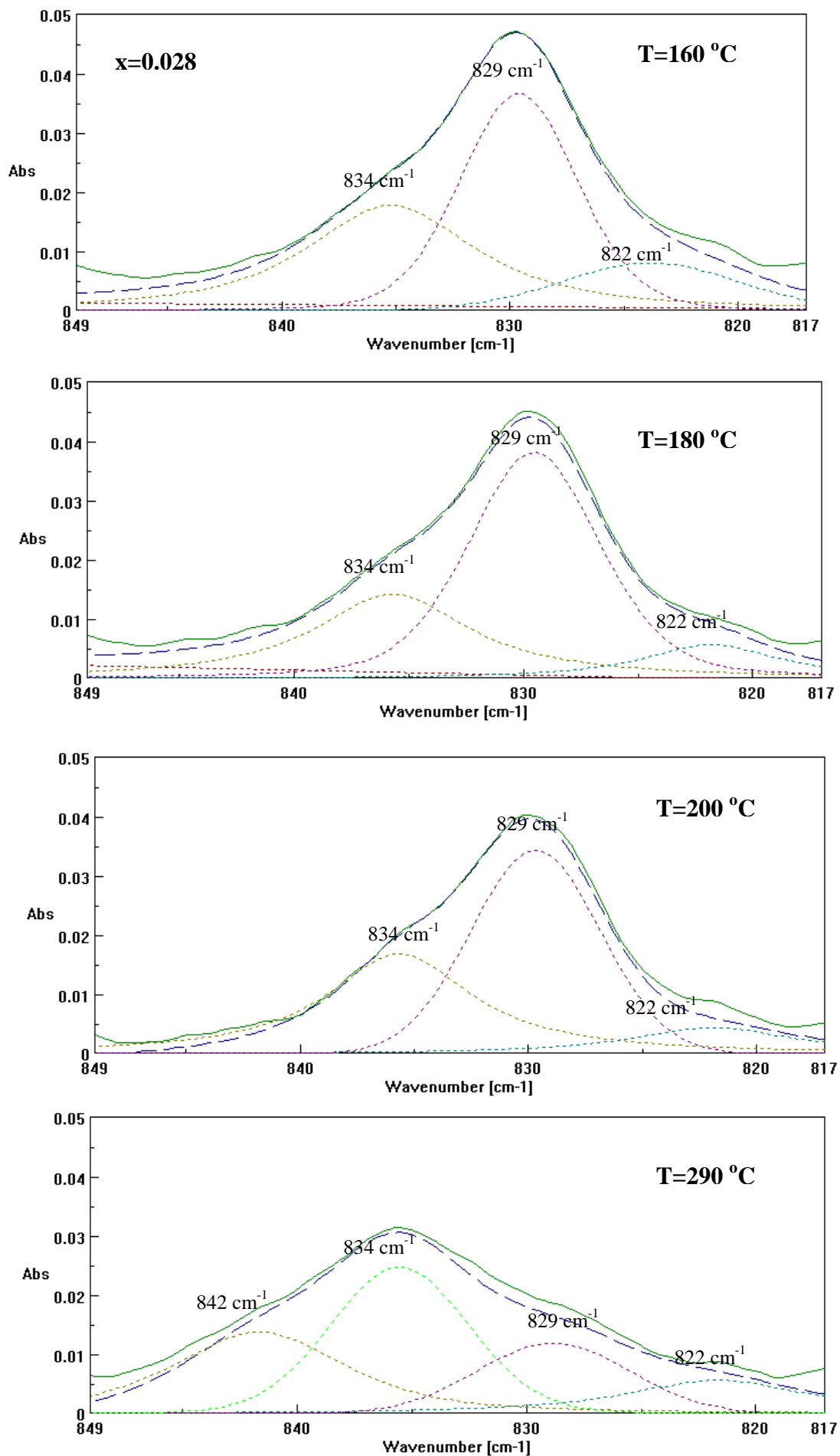
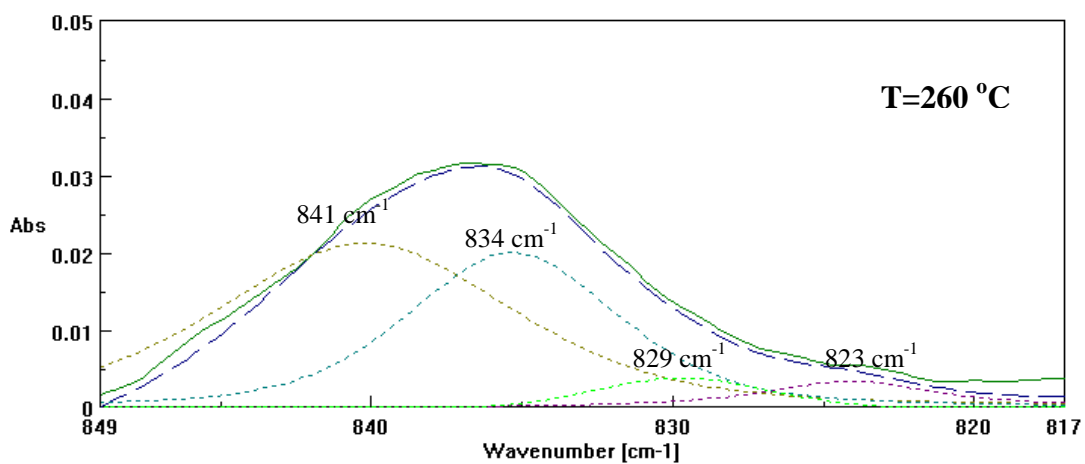
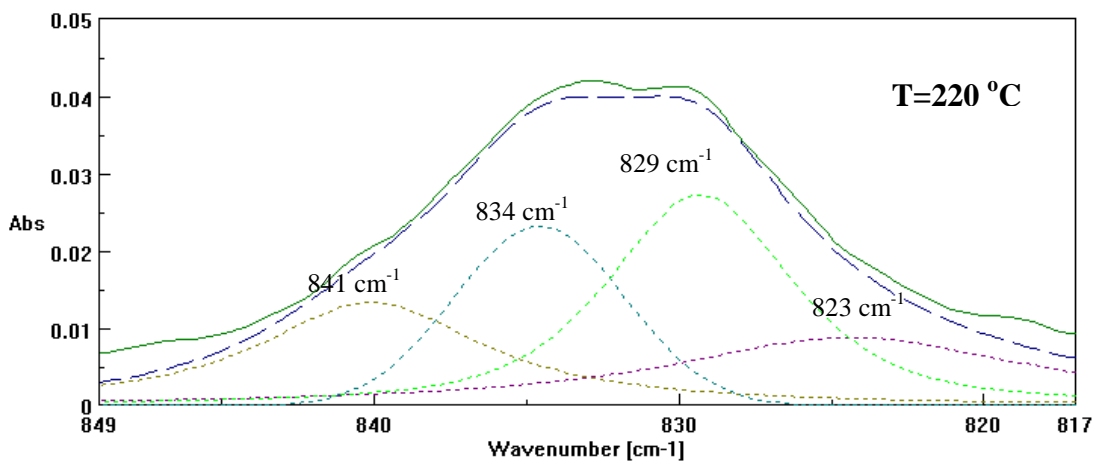
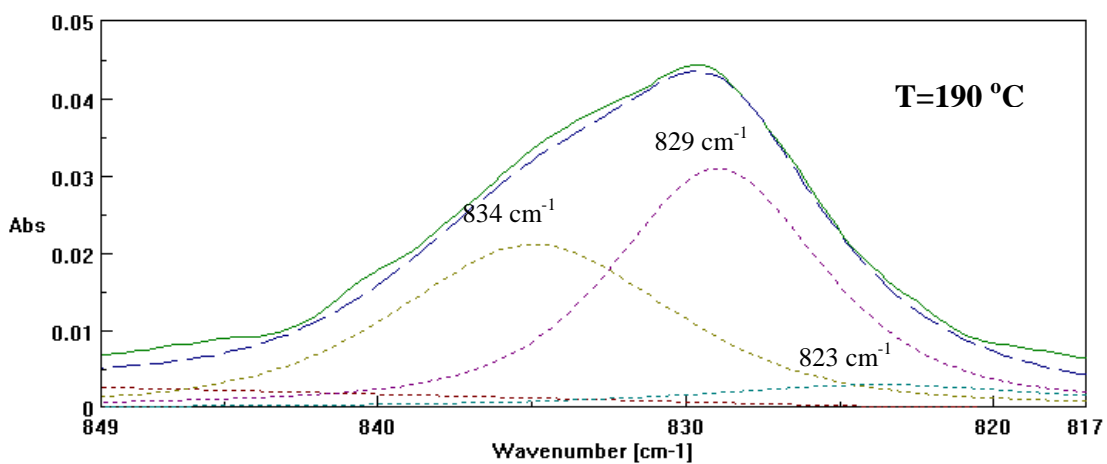
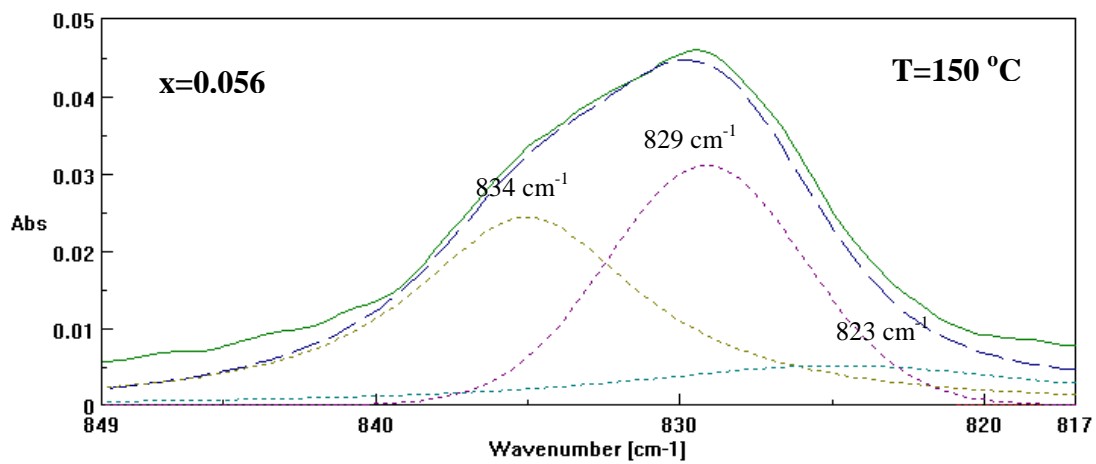


Fig. 3







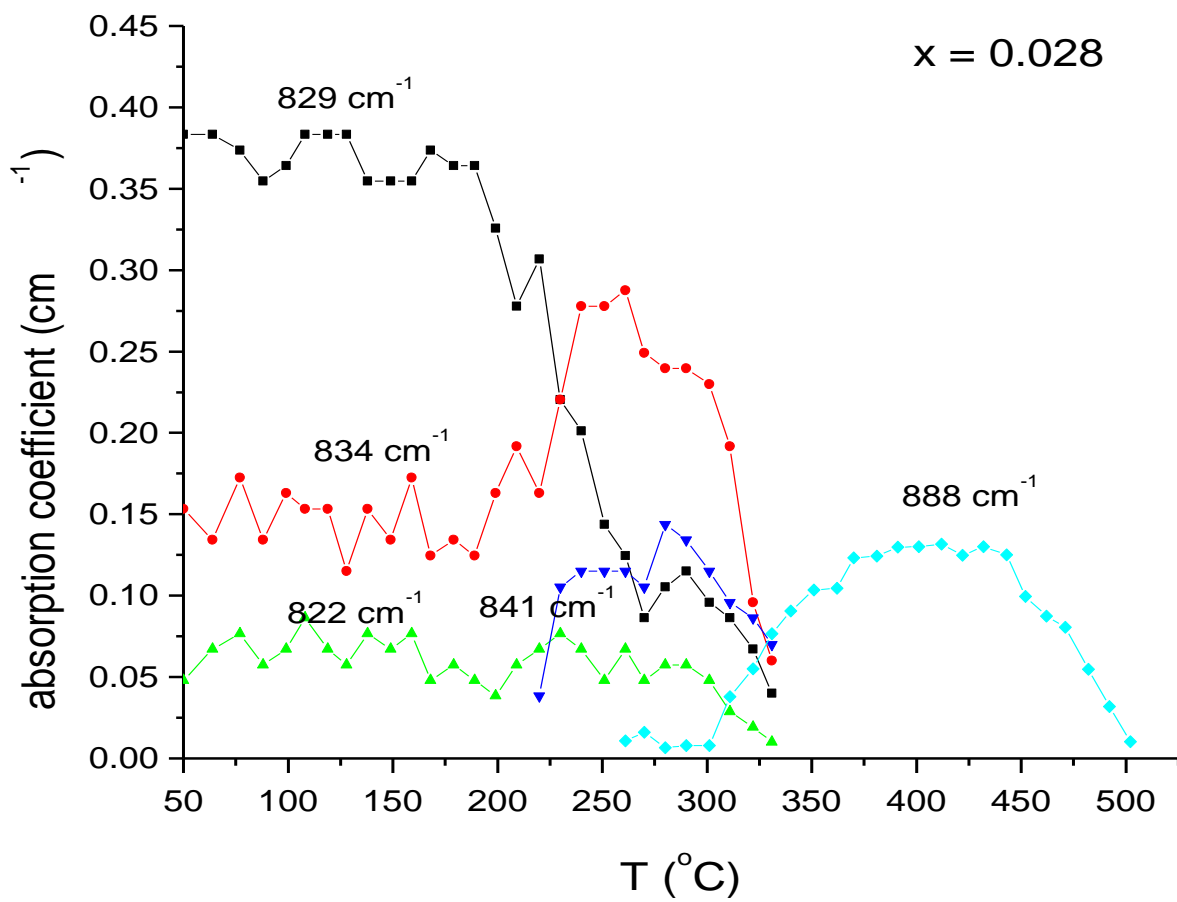


Fig. 5(a)

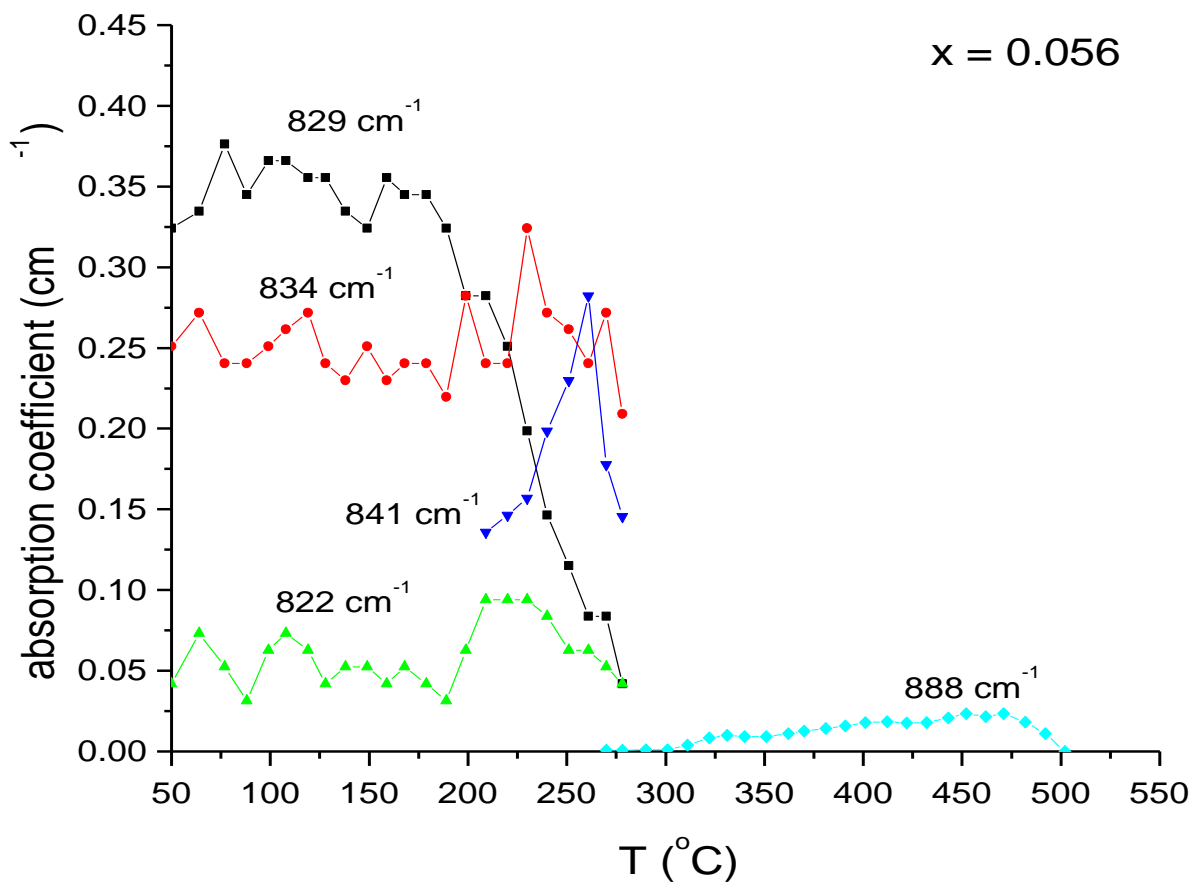


Fig. 5(b)

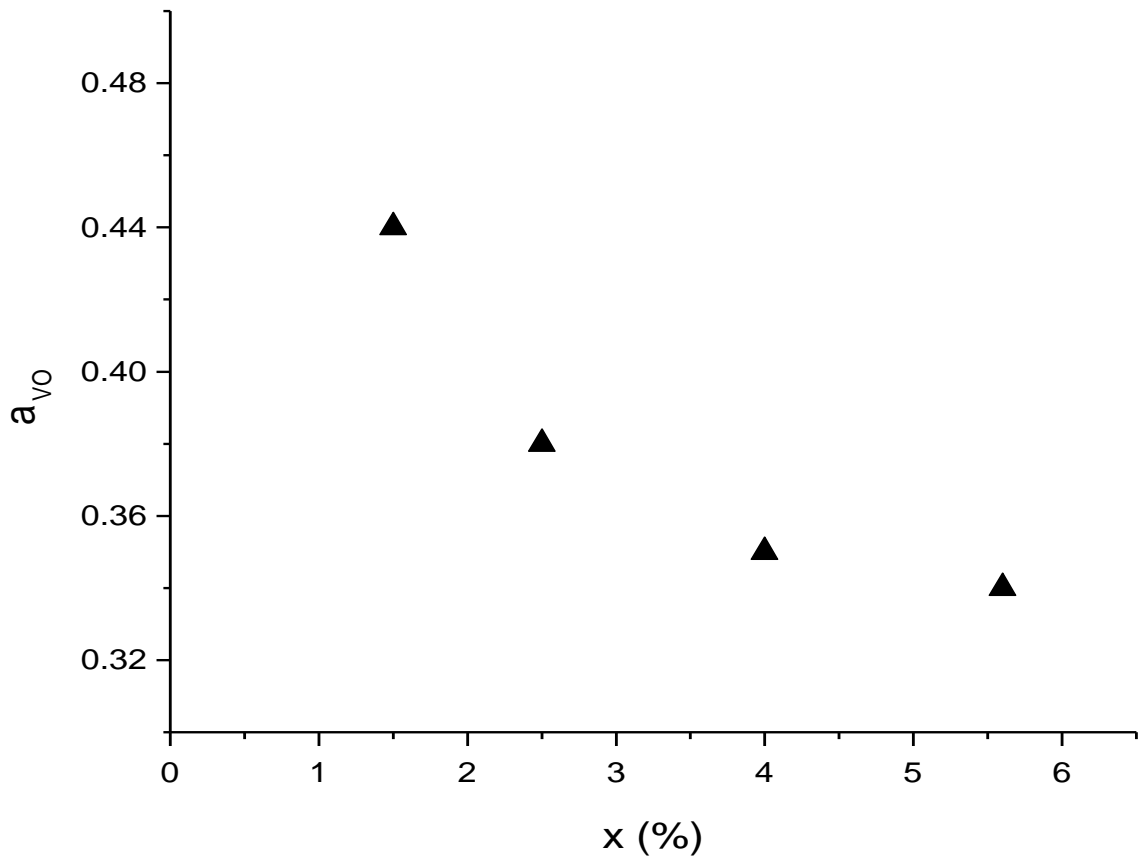
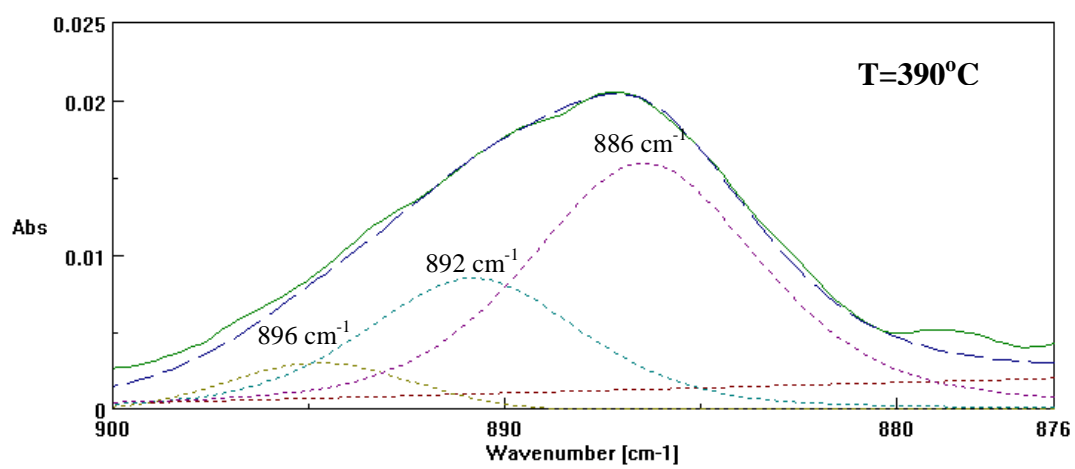


Fig. 6



**Fig. 7**

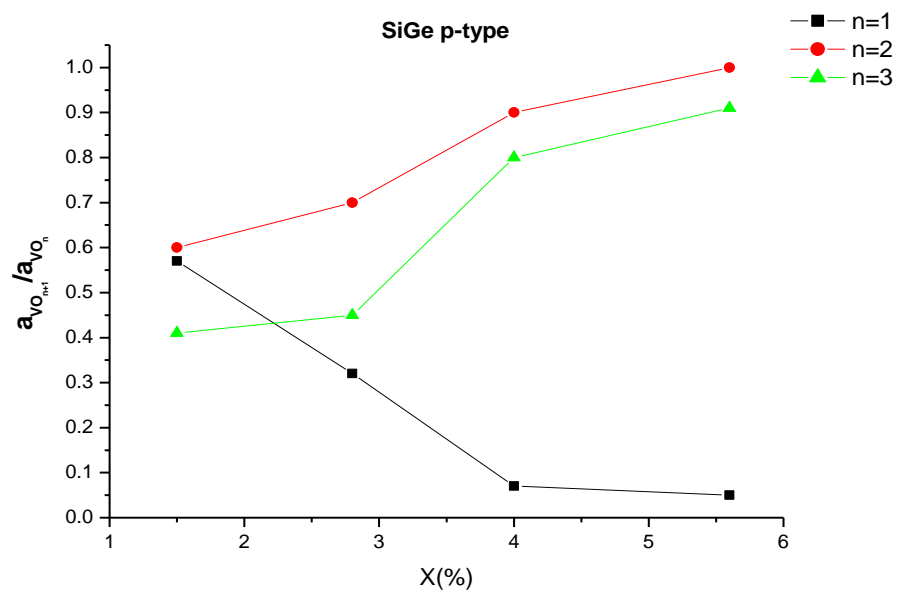


Fig. 8