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The Effect of Increased Methane Flow Rate on Electronic Correlation of Amorphous Silicon Carbon (a-SiC: H)

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Abstract

In this study, we report for the first time that the addition of methane (CH₄) flow rate in the p-type a-SiC: H layer greatly affects the electronic correlation in increasing the conversion efficiency of solar cells. The a-SiC: H p-type layer was grown using *Plasma Enhanced Chemical Vapor Deposition* (PECVD) on *Indium Tin Oxide* (ITO) substrate with various methane flow rates. The a-SiC: H p-type layer was characterized including the complex dielectric properties and the complex refractive index using *Ellipsometric Spectroscopy* (ES), while the surface roughness morphology was used *Atomic Force Microscopy* (AFM). In sample P-2 there is a change in the form of a decrease in the value of the refractive index $\langle n \rangle$ and the E_0 energy in the lower energy compared to the P-1 sample with a change of 0.3 eV, an increase in the optical gap and a decrease in the value of the real and imaginary dielectric function. While the influence of an increase in the carbon composition of the amorphous network order shows the addition of amorphous tissue disorder. Our results, show that the optical magnitude of the p-type a-SiC: H layer is not only affected by the amount of carbon in the film but also the hydrogen which is thought to contribute.

Keywords: a-SiC: H, ES, Flow rate, Methane, p-type, PECVD.

1. Introduction

The p-type layer of a-SiC: H is applied to the solar cell on top of silicon, the p-type layer in solar cells based on a-SiC: H p-i-n. As a light-receiving layer, p-type layer should be transparent so that the incoming photons more much, which means the carrier concentration increases [1-3]. In order for the p-type layer to be transparent and able to increase the concentration of the charge carrier, carbon is added when depositing the p-type layer which is made thinner. With the addition of carbon at the time deposited p-type layer, dangling bonds on the surface and become more transparent layers so that the percentage of photons that arrive at the intrinsic layer will increase [4-5]. Therefore, the composition greatly affect the optical gap p-type layer of a-SiC: H.

The optical gap width of the p-type a-SiC: H layer can also be obtained larger in the presence of carbon, besides that the presence of the amount of hydrogen also affects the optical gap increase, so it is often used as a transparent layer that is doped in solar cell applications, sensors, and electrolysis [6-8]. Increasing the width of the optical gap with the presence of carbon in the network layer of the p-type a-SiC: H followed by a worsening of its electrical properties and increased disorder [9-11]. The presence of carbon can increase the width of the state density in the tail region of the energy band, which can decrease the drift mobility thus worsening the electrical properties, whereas the reduction in disorder is thought to be due to the presence of trigonal C=C sp^2 in the sp^3 tetrahedral amorphous network [12-13]. The state density in the tail of the valence and conduction bands is reflected in the slope of the optical absorption curve so that it can be used to determine the electrical properties and amorphous semiconductor disorder. The unfavorable electrical properties are also thought to be related to structural characteristics such as a high number of voids or the formation of certain hydrogen bonds [14]. Therefore, it is necessary to know the structural characteristics and their relationship with the amorphous semiconductor material disorder which affects their electrical properties.

Information about the optical gap of the p-type a-SiC: H layer can be obtained from the optical absorption coefficient α in the visible region, while the optical absorption coefficient α can experimentally be found from the refractive index of the $N = n-ik$ complex as a function of energy [15-16]. Therefore, both the optical magnitude α and n as a function of energy needs to be known in the study of the optical characteristics of the p-type layer of a-SiC: H. This research will study the two optical quantities for the p-type layer a-SiC: H

deposition result by RF-PECVD method. The effect of variations in the flow rate of methane gas on these two optical quantities will be studied with data on the amplitude ratio $\langle \psi \rangle$ and the phase difference ratio $\langle \Delta \rangle$ between the p and s polarization light waves from the ellipsometric spectroscopy measurements.

2. Experiment Method

In this study, the p-type layer of a-SiC: H grown on *Corning glass 7059* substrate which has been prepared with *Indium Tin Oxide* (ITO). The PECVD technique used consists of two multi-chamber deposition chambers, each of which is specifically used to deposit p-type a-SiC: H layers as shown in Fig 1. In this condition, the filament temperature is only determined by the radiation heater temperature (substrate temperature). Silane gas (SiH₄) with a concentration of 10% in *hydrogen* (H₂) is used as the source gas. Used as a dopant gas *diborane* (B₂H₆) gas concentration of 10% in H₂ for the p-type dopant layer and the addition of *methane* (CH₄) as a p-type layer optimizations that are transparent and capable of increasing the concentration of charge carriers [17]. The growth parameters used are shown in Table 1.

Elipsometric spectroscopy (ES) parameters ψ and Δ (ie, the ratio of the amplitude and the phase difference between the reflected light polarized p and s, respectively) were collected on a 70° angle of incidence, the photon energy range between 0.6 and 6.5 eV using ellipsometric spectroscopy (V-VASE, J. A. Woollam Co.) with a rotating analyzer and compensator in *Singapore Synchrotron Light Source* (SSLS). In further analysis of the fitting of the measurement data, software is used *Woollam Complete Ease*, with the parameters used in accordance with the surface roughness of the measurement results P-1 and P-2 *Atomic Force Microscopy* (AFM). For each parameter of the dielectric function was evaluated with a combination of *Tauc-Lorentz models* (TL)/*Tauc-Lorntz+G* to determine the thickness, roughness, bandgap, and optical constants p-type layer of a-SiC: H [18].

The following equation is used to analyze the results of elipsometri spectroscopy measurements on the p-type layer of a-SiC: H [19].

1) Complex dielectric functions $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$ (ω = the angular frequency of the incident photon).

2) Refractive index $n(\omega) = \sqrt{\frac{1}{2}[\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} + \varepsilon_1(\omega)]}$

$$3) \text{ Extinction coefficient } \kappa(\omega) = \sqrt{\frac{1}{2} [\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} - \varepsilon_1(\omega)]}$$

$$4) \text{ Loss function } -Im[\varepsilon^{-1}(\omega)] = \frac{\varepsilon_2(\omega)}{[\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)]}$$

$$5) \text{ The reflectivity of normal incidence } R(\omega) = \frac{[n(\omega)-1]^2 + \kappa^2(\omega)}{[n(\omega)+1]^2 + \kappa^2(\omega)}$$

3. Result and Discussion

Measurement $\langle \psi \rangle$ and $\langle \Delta \rangle$ of ellipsometric spectroscopy for samples of P-1 and P-2 show in Fig 2 along with the results of data fitting. To support the optical and electronic analysis of each sample, obtained from the sample surface roughness of P-1 and P-2 as in Fig 3. which showed the surface morphology of P-1 and P-2 on $2 \times 2 \mu\text{m}^2$ film area. In the P1 and P-2 samples it is seen that they are very uniform across the samples. Where the small grain size was observed in samples of P-1 and the grain size is increased in samples of P-2. This is due to changes in the nucleation process and growth in the sample with the addition of the methane flow rate. The *root-mean-square* (RMS) surface roughness values of the samples obtained from AFM measurements were found to be 8.95 and 6.20 nm according to sample P-1 and sample P-2.

The p-type layer of a-SiC: H were measured at room temperature in the optical energy range 0.6-6.6 eV. From the results of the sample fitting P-1 and P-2 obtained information and parameters of the optical properties of materials, such as refractive index, dielectric constant, the absorption coefficient, thickness and roughness p-type layer of a-SiC: H. Furthermore, from the *complex dielectric function* $\langle \varepsilon_1 \rangle$ and $\langle \varepsilon_2 \rangle$ obtained *loss-function*, as well as *optical conductivity* $\langle \sigma_1 \rangle$ and from *refractive index* $\langle n \rangle$ and *extinction coefficient* $\langle k \rangle$ obtained *normal incident reflectivity* $\langle R \rangle$ of each sample [20].

3.1 Complex dielectric function $\langle \varepsilon_1 \rangle$ and $\langle \varepsilon_2 \rangle$

The dielectric function $\langle \varepsilon \rangle$ describes the optical and electrical properties of the material over the measurement energy range. Dielectric function consists of two components, namely the real $\langle \varepsilon_1 \rangle$ and imaginary $\langle \varepsilon_2 \rangle$. The real component $\langle \varepsilon_1 \rangle$ represents the polarization of the material due to the electric dipole which contributes to the atomic and electric polarization, while the imaginary component $\langle \varepsilon_2 \rangle$ represents the amount of light absorption in the material [21]. In Fig 4 the real component $\langle \varepsilon_1 \rangle$ shows the value of E_0 in sample P-1 of 2.94 eV and sample P-2 of 2.64 eV. Where there is a change in E_0 energy in sample P-2 changes in energy to be smaller than sample P-1 with a large change of 0.3 eV, this proves that at that energy P-

2 sample can absorb more energy than sample P-1 and ultimately to improve the performance of the p-type layer on the solar cell based p-i-n a-SiC: H. The same is true for the imaginary component $\langle \epsilon_2 \rangle$ the values of E_1 and E_2 which are characteristic of the excitability of each sample, showing that in sample P-2 the values of E_1 and E_2 change at a smaller energy than that of sample P-1.

3.2 Refractive index $\langle n \rangle$ and Extinction coefficient $\langle k \rangle$

The values of the complex refractive index $\langle n \rangle$ and $\langle k \rangle$ obtained through ellipsometric spectroscopic measurements represent the $\langle n \rangle$ value which represents the refractive index of the material and the $\langle k \rangle$ value which represents the extinction coefficient of material absorption and energy lost due to the scattering process [22]. Figure 5 shows the optical properties of the sample layer P-1 and P-2 for measurements at the same temperature on the substrate ITO. In the P-2 sample, the p-type a-SiC: H layer quality was quite good in terms of the lowest n value compared to the P-1 sample. At energy <3.0 eV in $\langle n \rangle$ sample P-2, there is a very sharp decrease compared to sample P-1, this shows that the maximum absorption rate obtained is greater for sample P-2 than for sample P-1 even though for each sample it is measured at the same substrate temperature. During deposition, the substrate temperature greatly affects the diffusion process of the deposited atoms on the substrate. In this case because the temperature of the substrate will cause the atoms of the surface of the substrate to vibrate and as a result, the distance between the planes stretches, making the insertion process easier.

In the extinction coefficient $\langle k \rangle$ in sample P-2, it is found that > 3.0 eV is a smaller value than in sample P-1, this indicates that the results of sample P-2 are denser than sample P-1. This shows the extinction coefficient tends to decrease with increasing flow rate of methane gas. Extinction coefficient curves obtained are in limited energy so that it will have an energy price that is owned by a second layer of p-type a-SiC: H. However, at energies > 1.2 eV, a more transparent p-type a-SiC: H layer is produced, this is evidenced by the value of $\langle k \rangle$ which is towards the negative, this is likely to occur saturation of the insertion process of atoms and the result is a layer that is not dense.

3.3 Loss-function $\langle -Im [\epsilon^{-1}(\omega)] \rangle$ and Normal incident reflectivity $\langle R \rangle$

Loss-function $\langle -Im [\epsilon^{-1}(\omega)] \rangle$ as a function of energy can be obtained from the imaginary component $\langle \epsilon_2 \rangle$ and Normal incident reflectivity $\langle R \rangle$ obtained from the real component

$\langle \epsilon_1 \rangle$ [23], as shown in Fig 6 for both P-1 and P-2 samples. The figure shows a shift in the curve $\langle -Im [\epsilon^{-1}(\omega)] \rangle$ to a higher energy at P-2 with increasing methane gas flow rate. The shift is due to the influence of the flow rate of methane gas, whereas here there is a relationship between a shift to a higher energy and an increase in carbon concentration. The optical gap of the a-SiC: H p-type layer can be obtained from the curve *Normal incident reflectivity* $\langle R \rangle$ by using the definition of energy E_g , namely the definition of energy at the moment *Normal incident reflectivity* $\langle R \rangle$ valuable >3.0 eV.

The band structure model of the p-type a-SiC: H layer in the results of this study is illustrated as in Fig 8 for samples P-1 and P-2. Increasing the flow rate of methane increase the amount of carbon in the p-type layer of a-SiC: H. N_H determining the concentration of hydrogen contained in the p-type layer of a-SiC: H obtained from the experimental results of hydrogen effusion. Increasing the flow rate of methane gas also increases the concentration of hydrogen in addition to the amount of carbon in the p-type layer of a-SiC: H. Therefore, the effect of the flow rate of methane gas on the optical quantities stated above is due to the influence of carbon and hydrogen. The optical magnitude of the refractive index $\langle n \rangle$ and the optical gap E_g will be related to the amount of hydrogen and carbon in the p-type layer as shown in Fig 8. The figure shows that both carbon and hydrogen have an effect on reducing the refractive index $\langle n \rangle$ and increasing the optical gap E_g . Most researchers attribute increasing the optical gap to increasing carbon concentration alone, but hydrogen also has an effect. Likewise with the reduced refractive index $\langle n \rangle$ which most researchers associated with an increase in carbon concentration, even though the deposition process uses methane gas as a carbon source.

4. Conclusion

The effect of variations in the flow rate of methane gas on the optical characteristics of the p-type layer a-SiC: H deposition results from the PECVD technique shows changes in the form of a decrease in the value of the refractive index $\langle n \rangle$ and the E_0 energy in sample P-2 changes in energy to a smaller one than the sample P-1 with a change of 0.3 eV, an increase in the optical gap and a decrease in the value of the dielectric function of the real and imaginary parts. Meanwhile, the effect of increasing carbon composition on the regularity of amorphous tissue shows the addition of amorphous tissue disorder. The magnitude of the optical layer of the p-type a-SiC: H is not only influenced by the amount of carbon in the film but also hydrogen which is estimated to have contributed.

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Figures caption

- Figure 1** :Schematic of p-type a-SiC: H deposition sample preparation
- Figure 2** :Experimental data (*solid curve*) and fittings (*point curve*) from $\langle\Psi\rangle$ and $\langle\Delta\rangle$ to (a) P-1, and (b) P-2. Obtained by measurement by angle 70° .
- Figure 3** :Surface roughness (a) P-1 and (b) P-2. Measurement results with AFM.
- Figure 4** :(a) Real part $\langle\epsilon_1\rangle$, and (b) imaginary part $\langle\epsilon_2\rangle$. From the dielectric function for P-1 and P-2 sample a-SiC: H.
- Figure 5** :Complex refractive index (a) $\langle n\rangle$ and (b) $\langle k\rangle$ for samples P-1 and P-2 sample a-SiC: H
- Figure 6** :(a) Loss-function and (b) Reflectivity for samples P-1 and P-2 sample a-SiC: H.
- Figure 7** :Possible band-structure scheme in P-1 and P-2. E_F denotes fermi level. Thickness of arrows qualitatively indicates strength of the transitions

Figure 1

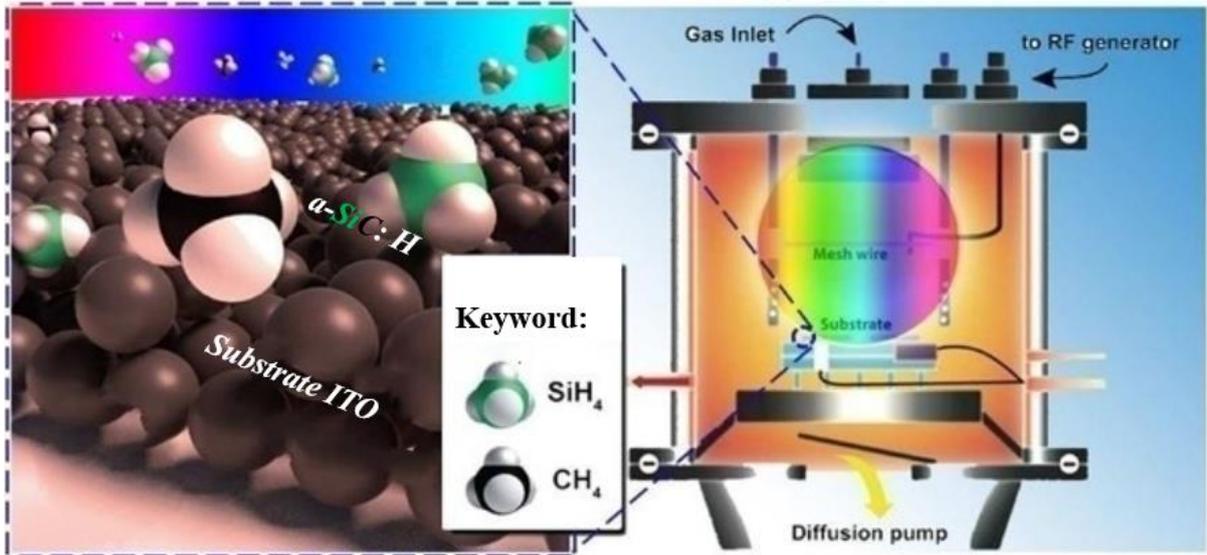
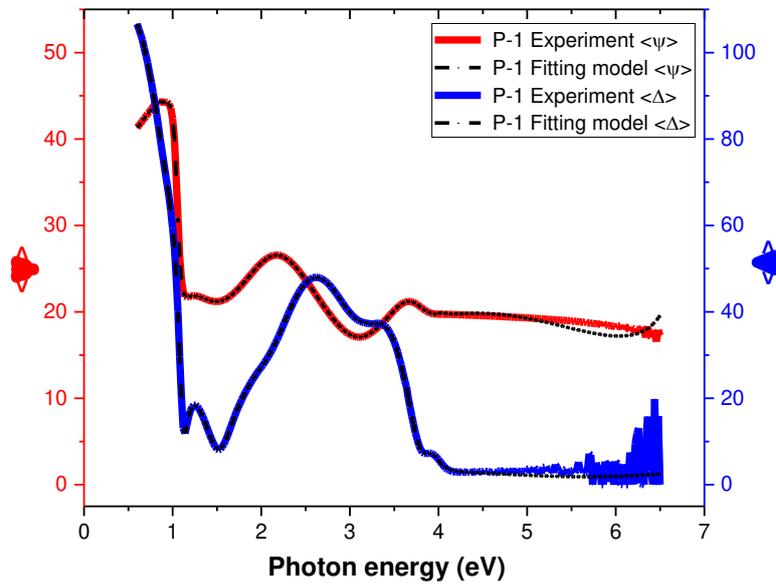
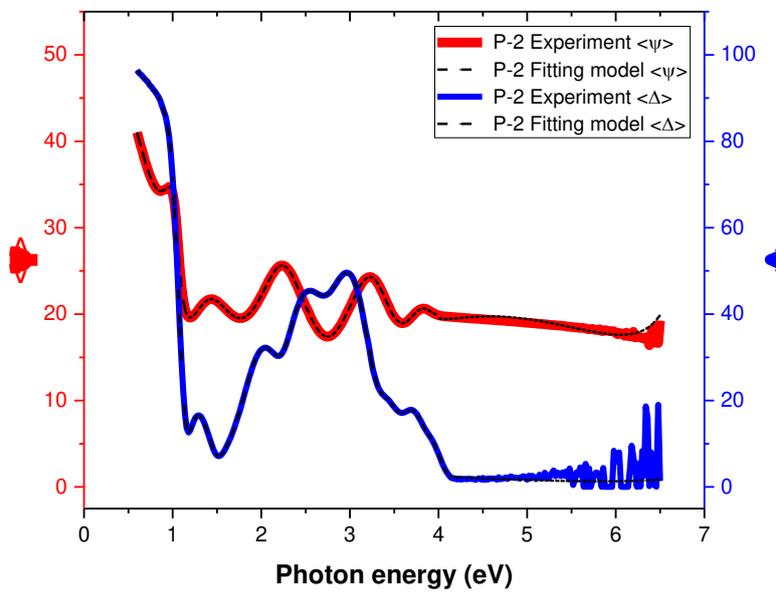


Figure 2

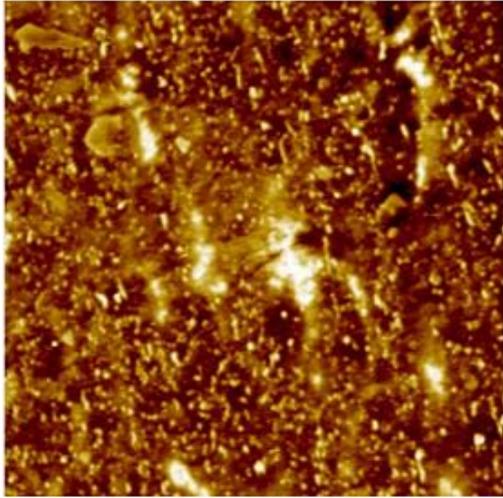


(a)

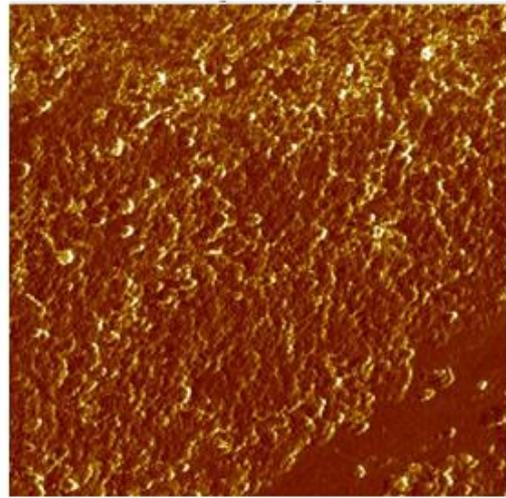


(b)

Figure 3

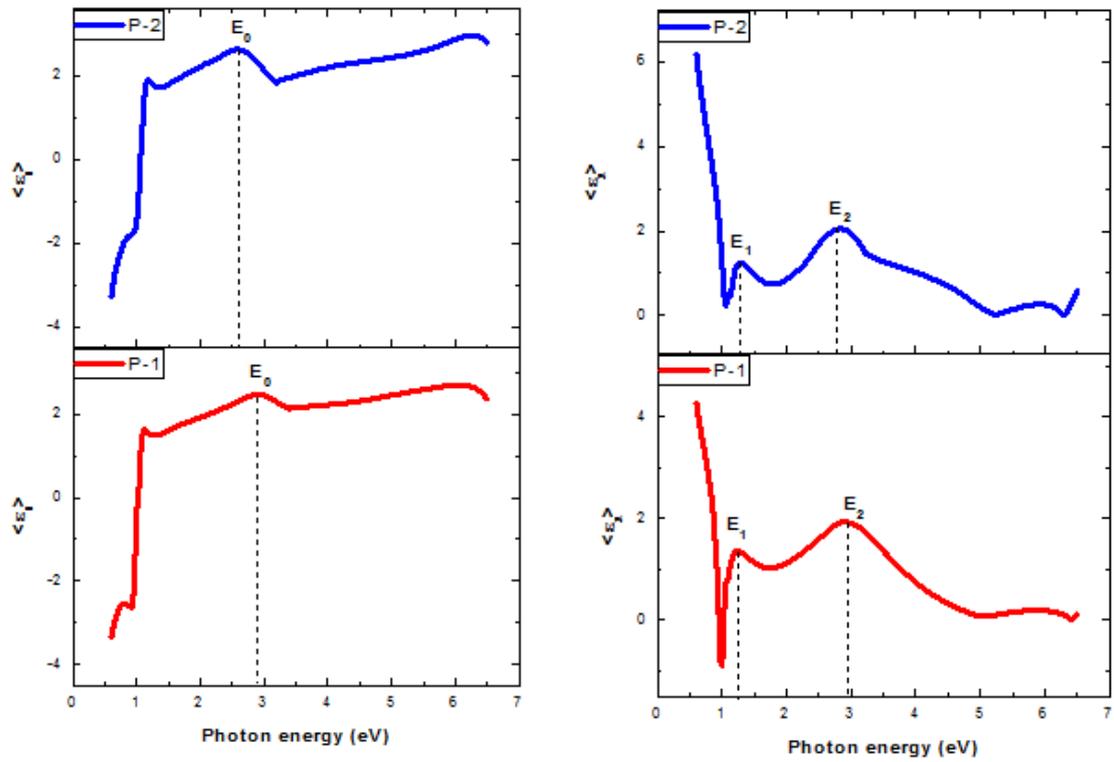


(a)



(b)

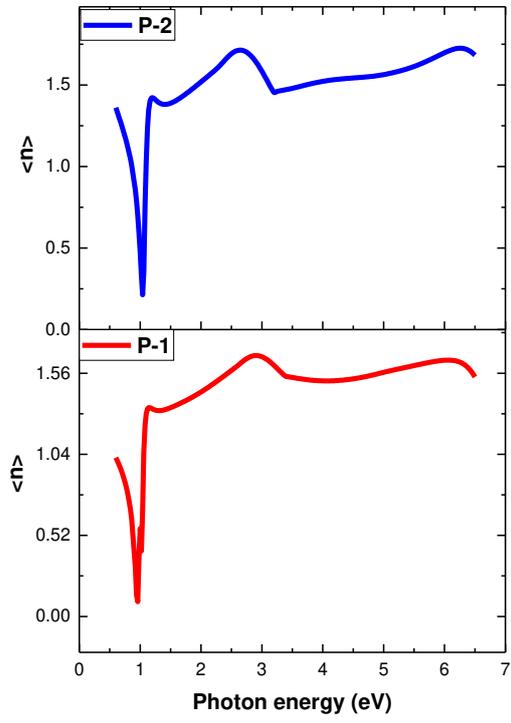
Figure 4



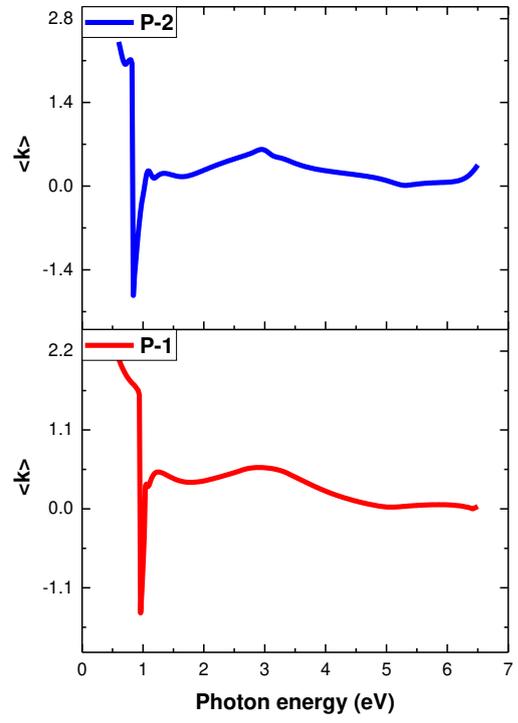
(a)

(b)

Figure 5

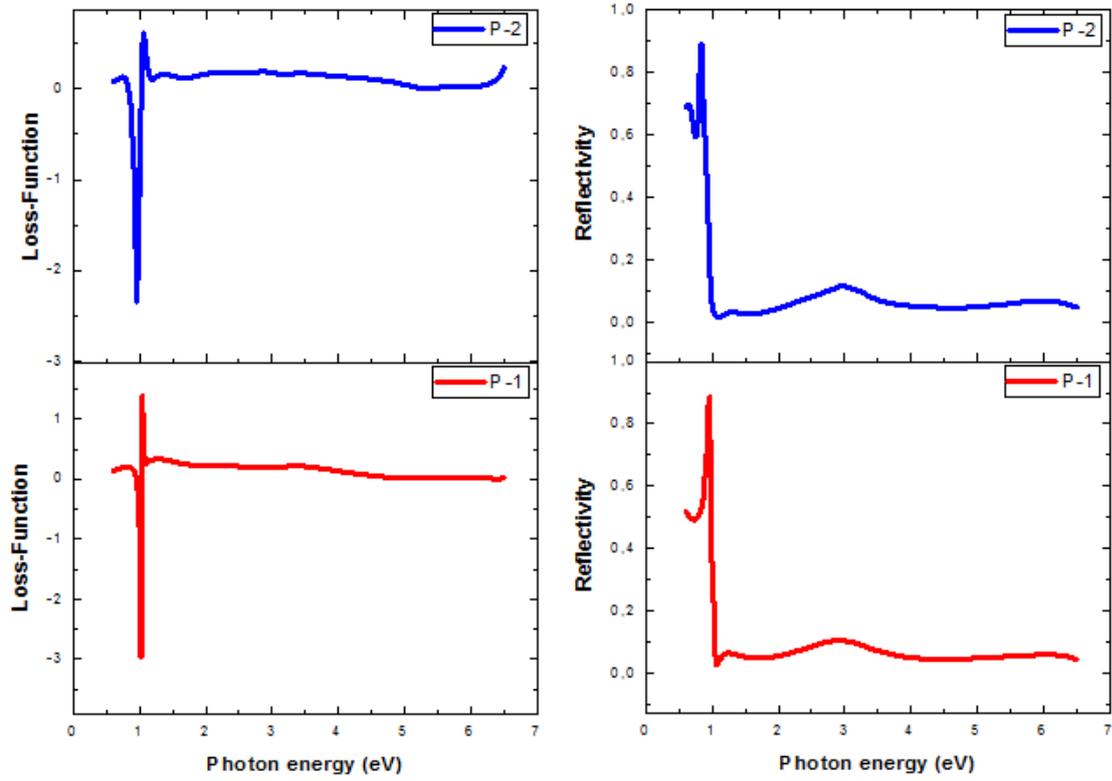


(a)



(b)

Figure 6



(a)

(b)

Figure 7

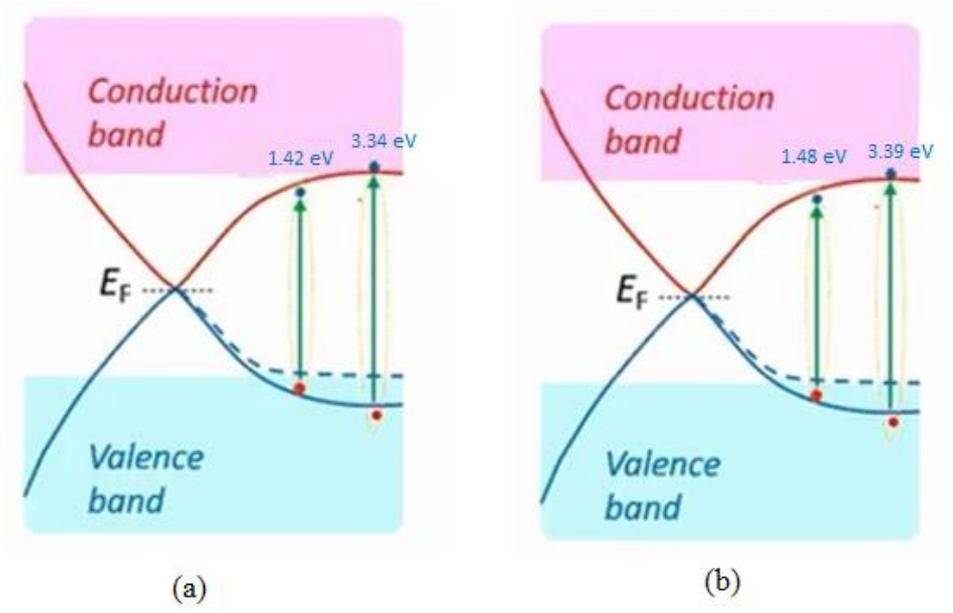


Table 1. Parameters for the deposition of the p-type layer of a-SiC: H

Deposition parameters	P-type layer of amorphous silicon carbon (a-SiC: H)	
	P-1	P-2
Flow rate SiH ₄	20 sccm	20 sccm
Flow rate B ₂ H ₆	2 sccm	2 sccm
Flow rate H ₂	20 sccm	20 sccm
Flow rate CH ₄	10 sccm	20 sccm
Power RF	5 Watt	5 Watt
Temperature	210°C	210°C
Pressure	4800 mTorr	4800 mTorr
Time	10 Minute	10 Minute

Author declaration

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Potential conflict of interest exists:

We wish to draw the attention of the Editor to the following facts, which may be considered as potential conflicts of interest, and to significant financial contributions to this work:

The nature of potential conflict of interest is described below:

No conflict of interest exists.

We wish to confirm that there are no known conflicts of interest associated with this publication and there has been no significant financial support for this work that could have influenced its outcome.

2. Funding

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[LPDP]

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We confirm that we have given due consideration to the protection of intellectual property associated with this work and that there are no impediments to publication, including the timing of publication, with respect to intellectual property. In so doing we confirm that we have followed the regulations of our institutions concerning intellectual property.

4. Research Ethics

We further confirm that any aspect of the work covered in this manuscript that has involved human patients has been conducted with the ethical approval of all relevant bodies and that such approvals are acknowledged within the manuscript.

IRB approval was obtained (required for studies and series of 3 or more cases)

Written consent to publish potentially identifying information, such as details or the case and photographs, was obtained from the patient(s) or their legal guardian(s).

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2. Drafting the work or revising it critically for important intellectual content; AND
3. Final approval of the version to be published; AND
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1. <i>Soni Prayogi</i>	 _____	13/02/2021
2. <i>Darminto D</i>	 _____	13/02/2021

Figures

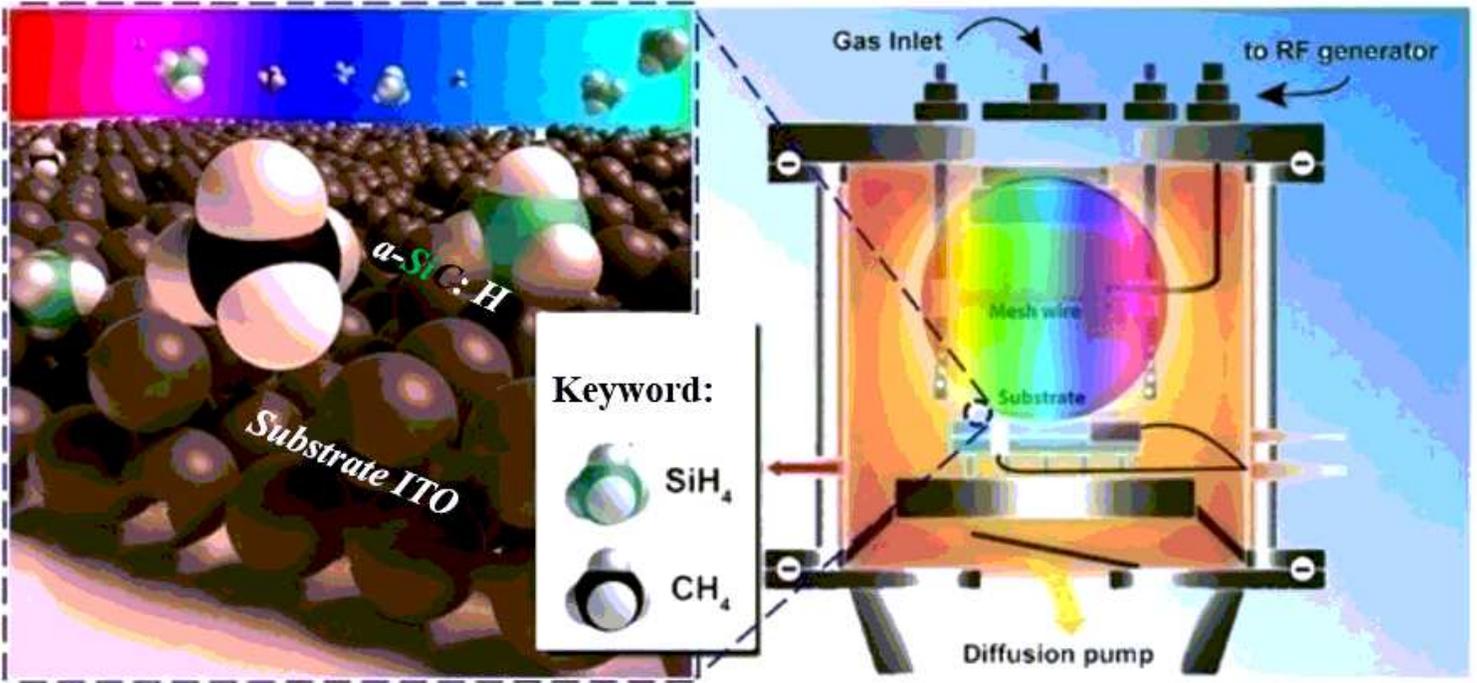


Figure 1

Schematic of p-type a-SiC: H deposition sample preparation

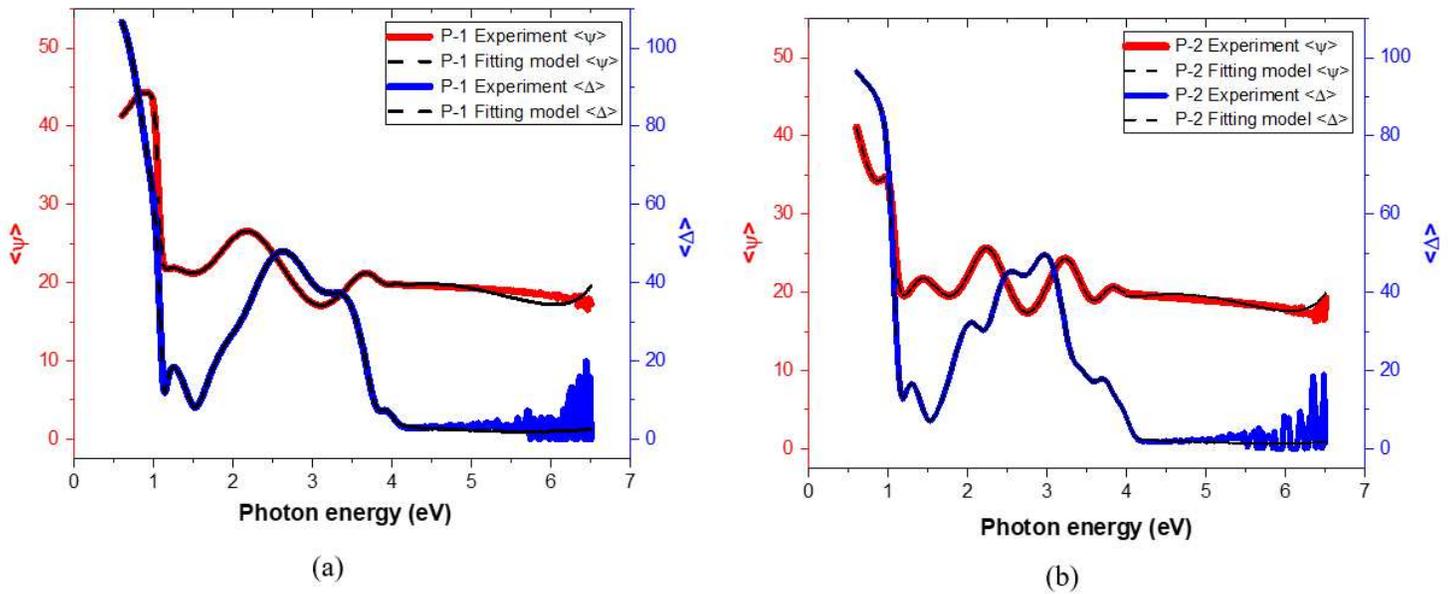
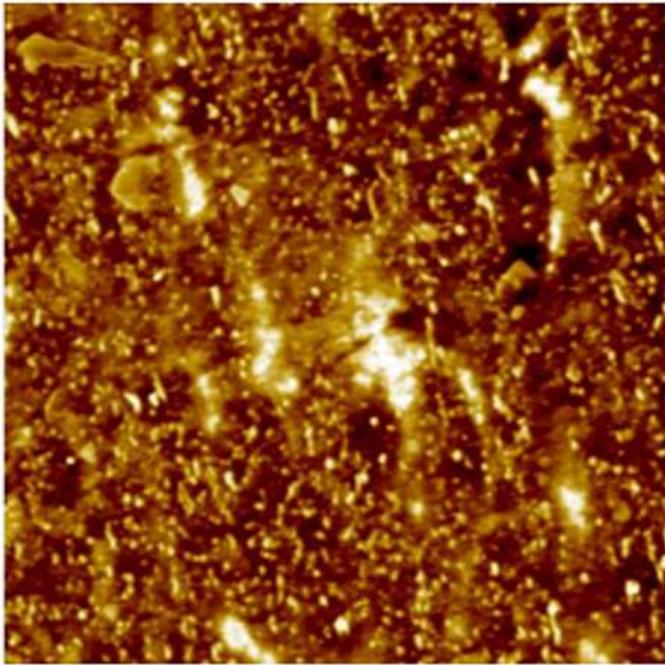
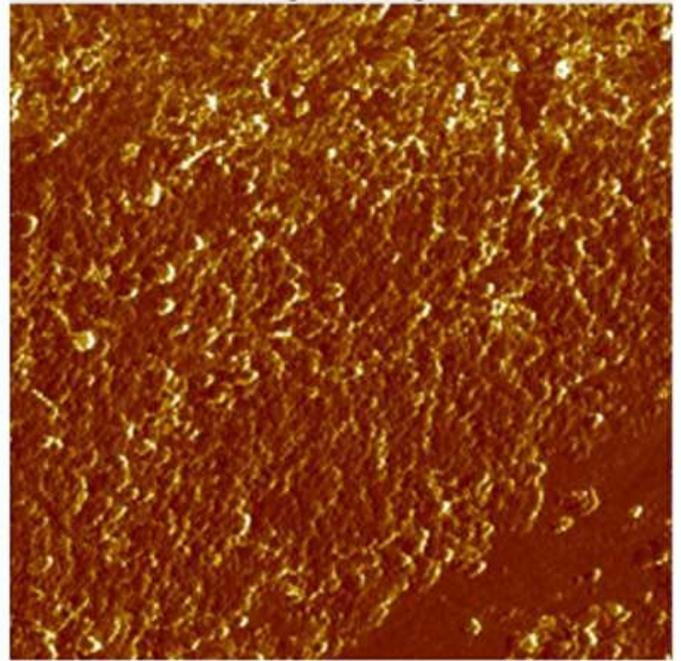


Figure 2

Experimental data (solid curve) and fittings (point curve) from $\langle \Psi \rangle$ and $\langle \Delta \rangle$ to (a) P-1, and (b) P-2. Obtained by measurement by angle 70°.



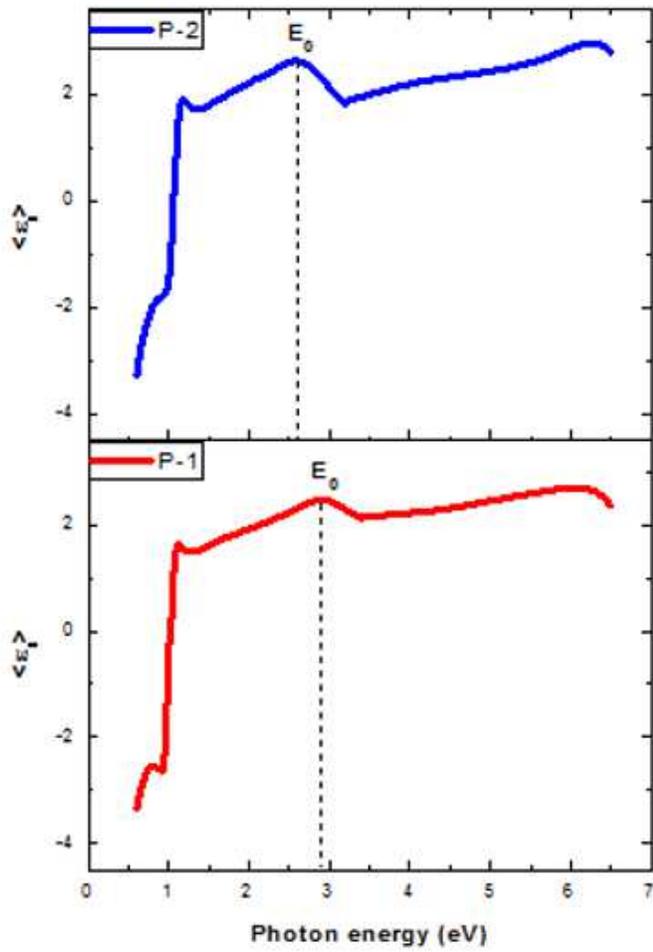
(a)



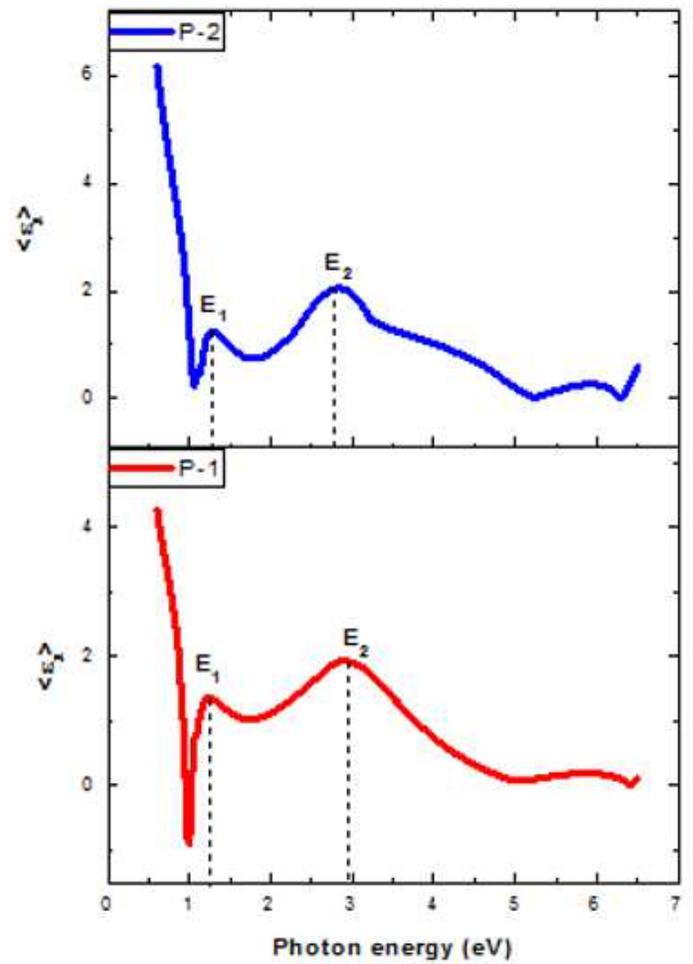
(b)

Figure 3

Surface roughness (a) P-1 and (b) P-2. Measurement results with AFM.



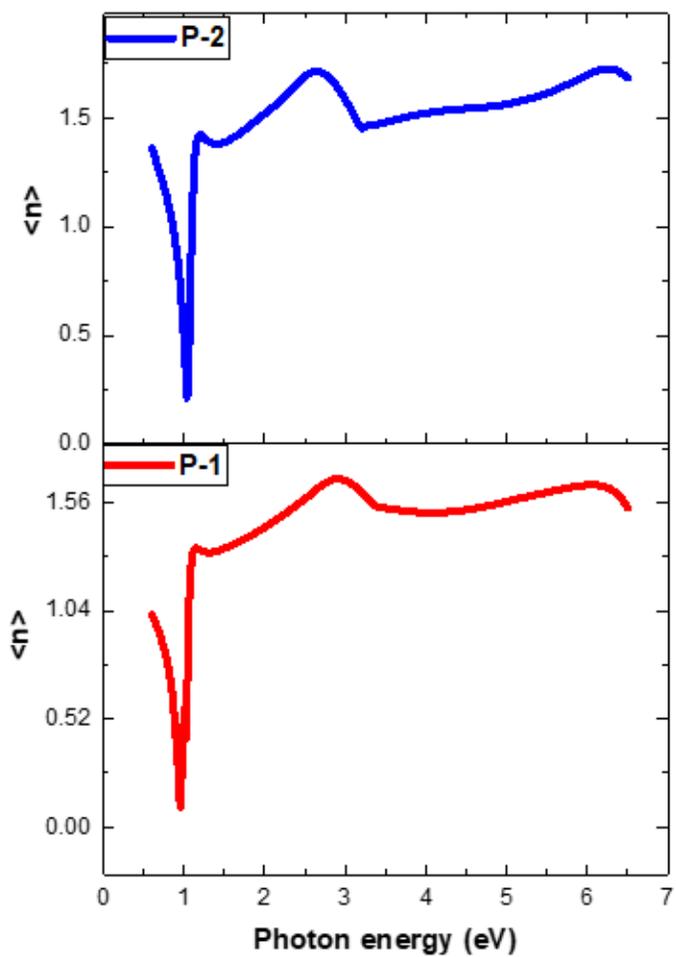
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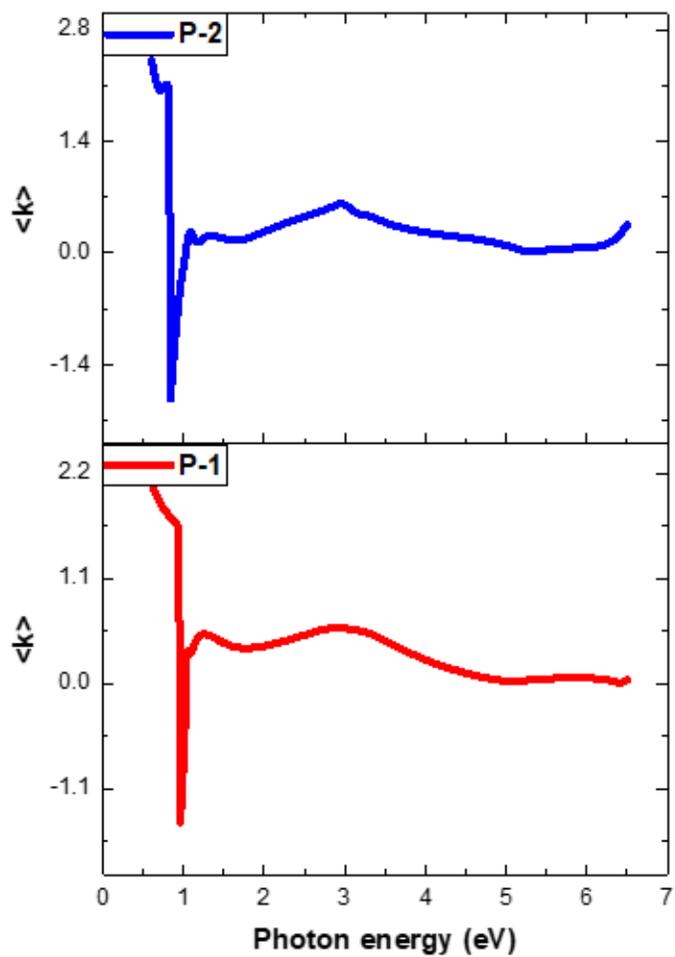
(b)

Figure 4

(a) Real part $\langle \epsilon_1 \rangle$, and (b) imaginary part $\langle \epsilon_2 \rangle$. From the dielectric function for P-1 and P-2 sample a-SiC:H.



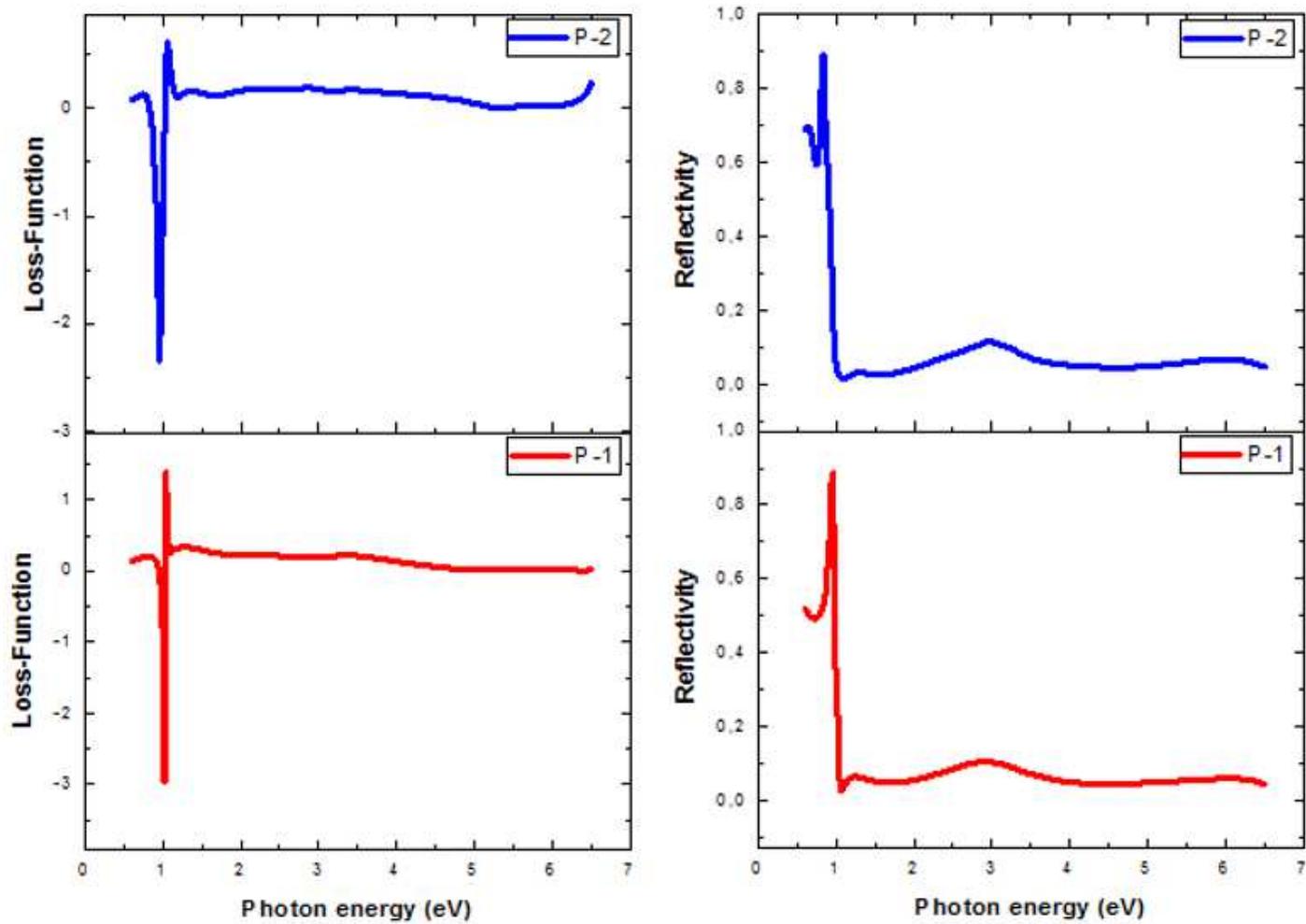
(a)



(b)

Figure 5

Complex refractive index (a) $\langle n \rangle$ and (b) $\langle k \rangle$ for samples P-1 and P-2 sample a-SiC: H

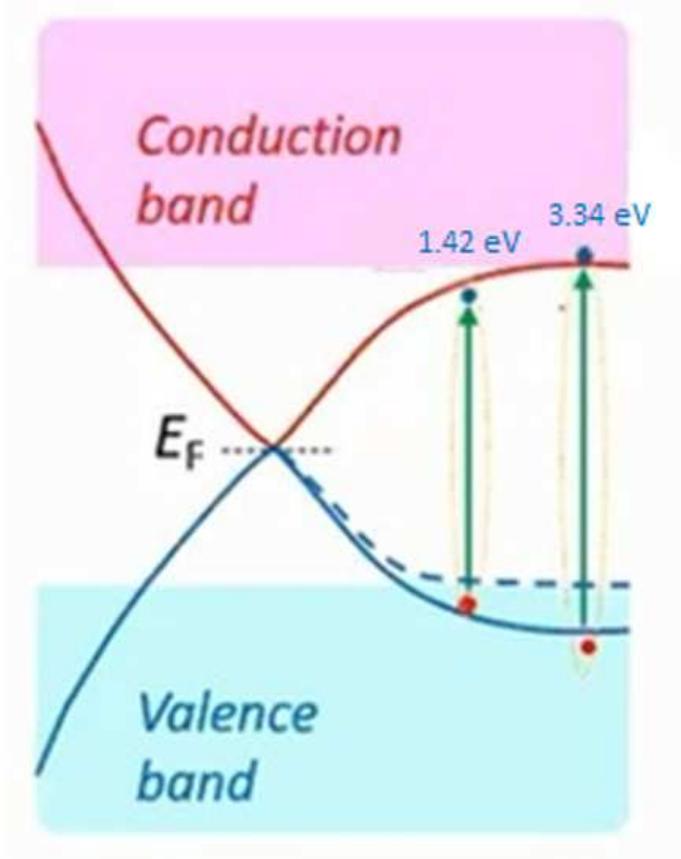


(a)

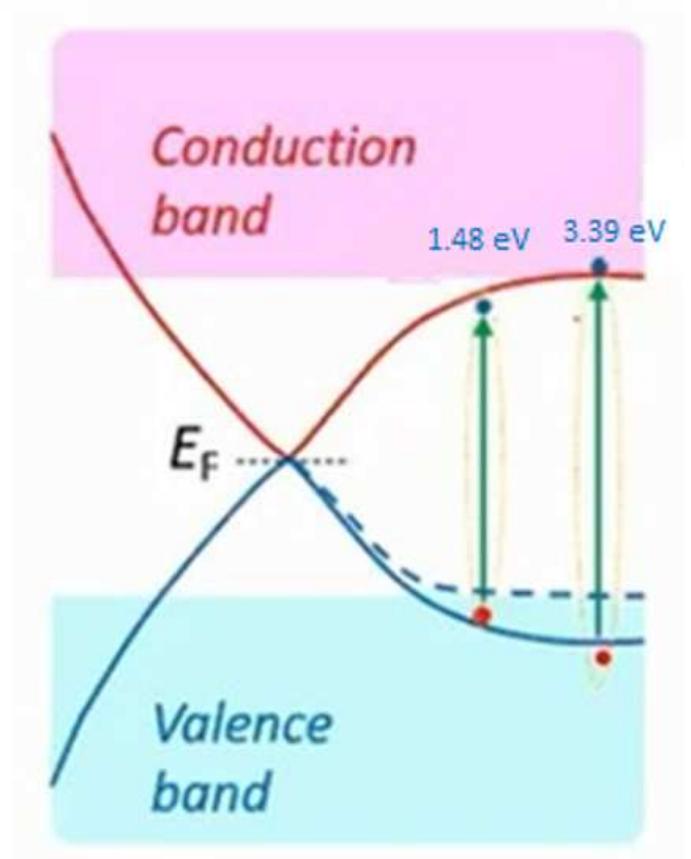
(b)

Figure 6

(a) Loss-function and (b) Reflectivity for samples P-1 and P-2 sample a-SiC: H.



(a)



(b)

Figure 7

Possible band-structure scheme in P-1 and P-2. E_F denotes fermi level. Thickness of arrows qualitatively indicates strength of the transitions