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Probing the Nature of Annealing Silicon Carbide Samples for Solar Cell

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Abstract

SiC powder preparation using Sol-Gel method. The size of nano-particles grows as the temperature exceeds 900° C. Size of probable agglomerations produced, is approximately less than 50nm. The surface is suitable to be used for dye solar cells. SiC emission occurs at wavelength area of 11.3μm or wave number area of 884.95 cm^{-1}. In this paper probing the nature of annealed SiC samples in mixture, sintered, burned, and washed with Si, being removed. We can conclude that the efficiency in trapping solar energy increases.

Key words: *Amorphous, Mixture, Nanostructure, Thin film, XRD.*

Introduction

Today, nano-materials and nanostructures are not only the forefront of the hot researches on the fundamental material, but also have entered slowly and intrusively into our daily lives .In recent years, the dye –sensitized nano-structured solar cells (DNSC) based on nanostructure metal oxide films have attracted much attention to themselves .The electrons and holes produced by light need to move on a shorter path to prevent the charge recombination greatly [1,2].

A .Losses due to reflection.

B .Recombination dissipation,

C. Loss due to series and parallel resistance.

Three approaches to curb the first two loss mechanisms: [3]

A. Increased number of energy levels, B. trapping hot carriers before normalization, C. generating pairs of electron - hole per high energy photons or producing a higher energy carrier pair with more than a low-energy photon.

Infrared spectroscopy is carried out, based

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on the radiation absorption and probing vibration mutations of molecules and ions. This method is employed as a powerful and advanced method in determining structures and measuring chemical species. Interaction of infrared radiation would result in modification of vibration energy of bonding in molecules in the sample, which nominates it as an appropriate method in identification of functional groups and the molecular structure. If the molecular dipole moment is changed during the vibration, Infrared energy absorption would occur. In electromagnetic spectrum, the region between 0.8 and 400 micrometers belong to infrared, but the region used for chemical analysis, is between 0.8 to 50 micrometers.

In order to obtain qualitative identification of an unknown sample, infrared spectrum of the sample is drawn based on the functional groups and existing molecular bonds, and by referring to relevant tables, which provides vibration position of different bonds or IR spectra of objects, wavelength or wave number of groups and bonds would be identified. One of the characteristics of FTIR is that the entire wavelength of the considered spectral region is simultaneously emitted on the sample. While in dispersive methods, only a small number of wavelengths reached the sample at one time. Therefore, the speed, resolution and signal-to-noise ratio in Fourier transform method is significantly better than the conventional IR methods. In brief, the qualitative and quantitative identification of organic compounds containing Nanoparticles, determination of functional group types and its molecular bonds, are FTIR objectives [4].

Experimental

Material

The reason why Sol-Gel Method is employed in the production of SiC Nano-powder, refers to factors such as : achieving high purity, increasing chemical activity, being needless of applying complex equipments, enhancing the functionality in Sintering materials, attaining high production capability, enabling control over properties and morphology, enabling synthesis at molecular level, enabling the production of very small particles with united diameter, enabling the production of particles with manageable and very high specific surface area, reducing the number of un-reacted materials in the final product [5].

In sol-gel method, in order to synthesize SiC nanopowder, when drying procedure is complete, Samples are powdered and are annealed at a temperatures of 500, 700, 900 and 1000° C. the process of annealing samples was done in Chemical vapor deposition (CVD) furnace, in air atmosphere with a thermal gradient of 5° C per minute. In order to probe particle shapes and for surface analysis of structures, Scanning Electron Microscope is used [6].

1. Radiation-absorption analysis using FTIR

C-C bond has an absorption frequency of 1200 cm^{-1}, double bond of C = C has an absorption frequency of 1650 cm^{-1} and triple bond of C = C has an absorption frequency of 2150 cm^{-1}. The bending motion is easier than stretch motion. For example, bending C-H is assigned to the area of 1340 cm^{-1} and stretching C-H is assigned to the area of 3000 cm^{-1}. Hybridization type also affects the absorption frequencies, so that the bonds power are respectively SP> SP2> SP3.

In the Range of $K = \lambda^{-1} = 600\ cm^{-1}$ to 1400 cm^{-1} ,due to limited amount of absorbed energy and the bending vibration of absorbed energy, most molecular Bonds are complex and crowded and therefore identification of entire absorption bonds in this region would be difficult. In other words, there is a unique pattern in this region [7].

Absorption bonds in the region of $K=\lambda^{-1}=600\ cm^{-1}$ to 1400 cm^{-1} , have more absorbed energy which is mostly because of stretching vibration in stronger bonds.

FTIR spectrum for SiC nanopowder, annealed at temperatures of 500°C, 700°C, 1000°C using (FTIR, SHIMADZU 8400S, JAPAN) suggests:

A – In the wave number $K=\lambda^{-1}=478.31\ cm^{-1}$, as the temperature increases, absorption amount is reduced. (From 90% in 500°C to 27% at 1000°C). On the other hand, in the absorption frequency or wave number, siloxane bond (Si-O-Si) is observable. This bond is the result of hydrolysis reactions and condensation of silicon alkoxide.

B - SiC emission occurs at wavelength area of 11.3μm or wave number area of 884.95 cm^{-1}. [3] Comparing these spectra we'll realize that in $K=\lambda^{-1}=825.48\ cm^{-1}$, there is a Si-C bonding which is a result of bonding among carbon atoms in acetic acid and ethanol with the Si bond in hydrolyzed and condensate Tetraethyl orthosilicate liquid ($SiC_8H_{20}O_4$). Moreover, by comparing spectra, we can conclude that as the temperature increases, the amount of absorption has increased due to SiC formation.

C–In $K=\lambda^{-1}=1087.78\ cm^{-1}$, in a range of 500°C to 700°C due to the double bond of C=O, absorption increases. However in the range of 700°C to 1000°C as temperature is increased, due to the formation of single bond C-O, the absorption is promptly reduced. In this absorption frequency, at all temperatures stated, Si-O bond is identifiable which is because of hydrolysis reaction and condensation of the silicon aloxides.

D-In $K = \lambda^{-1} = 2337.56\ cm^{-1}$, absorption bonds have more energy, which is generally because of stretching vibration of strong bonds. (Group frequency region).

At $K=\lambda^{-1}=1380.94\ cm^{-1}$ C-C and C-O bonds, the wave number of $K=\lambda^{-1}=1535.23\ cm^{-1}$ double bonds of C = C, in absorption frequency $K=\lambda^{-1}=2923.38\ cm^{-1}$ C-H bonds are identifiable.

2. Probing the nature of annealed SiC samples

in different states

A - Mixture:

With a review on the mixture of Si and C using XRD we'd come to this conclusion that, at lower temperatures the biggest proportion of Si phase is restored. However, at this temperature, CNT or carbon nano-tubes will also be restored. (Figure1). These nano-tubes are characterized by high efficiency in trapping solar energy, as light collector and transmitter. CNTs have excellent electrical properties, and play different roles in nano-structured solar cells. They could also be employed as transparent electrode in nano-structured solar cells.

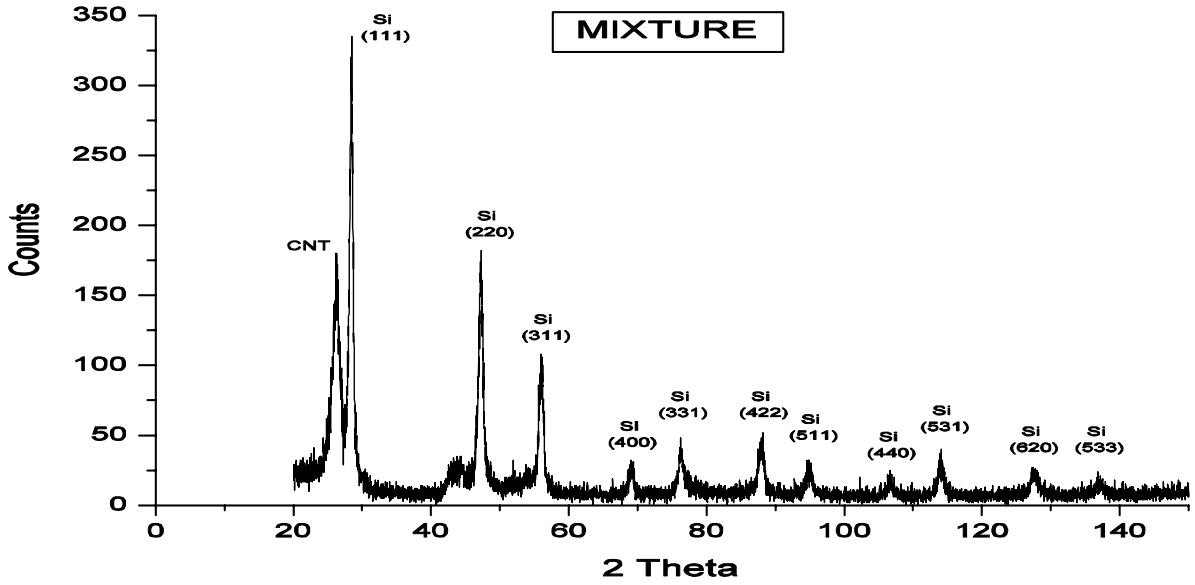

Figure 1. X-Ray Diffraction - Mixture

B - Sintered:

By sintering Si and C, and by placing the sample at 1200 °C for 2 minutes, we'll realize that in addition to restoring Si and CNT, silicon carbide is also restored. (Figure 2), But with reduction in their height, their width is reduced which means that according to Debye - Scherrer equation, particle size has increased. The reduction in resulting peaks intensity indicates rapid weakening in formation of Si, CNT due to the Sintering at 1200 ° C.

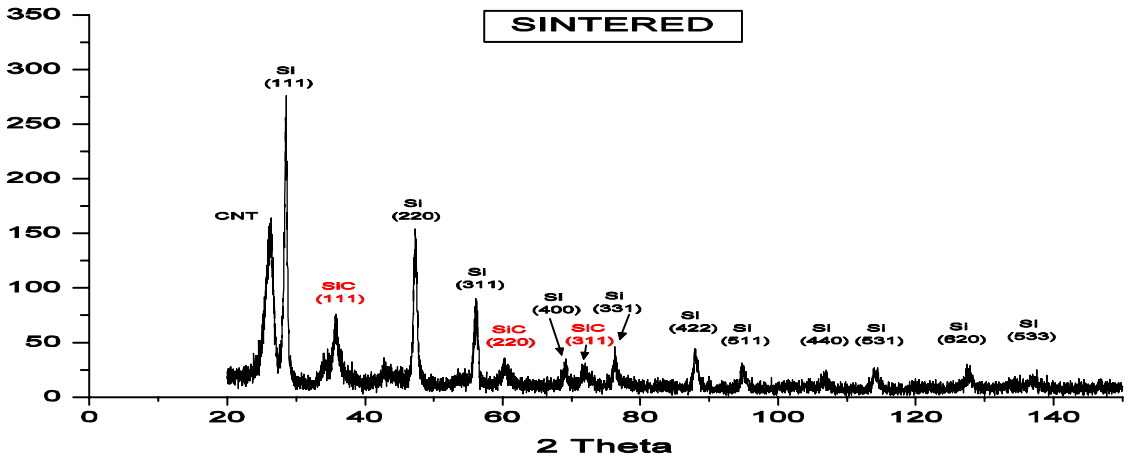

Figure 2. X-Ray Diffraction –sintered 2 min at 1200°C.

C - Burned:

By burning the sample for 2 hours at 700° C, we'll realize that the CNT phase is removed and only Si and SiC phases are restored. (Figure 3). In other words, sample efficiency in trapping solar energy lowers. However, the peak intensity of Si and SiC formation has increased. In conclusion, by burning the sample, we'll understand that Si and SiC formation rate increases, and also due to the increase in peak height, particles tend to turn into nanostructured particles.

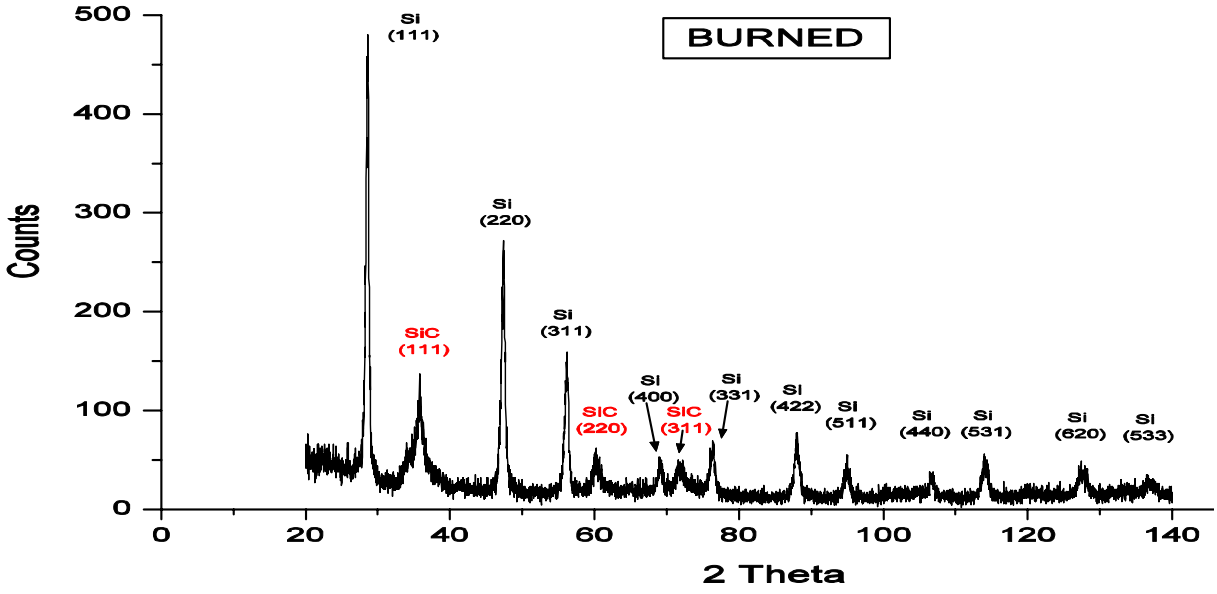

Figure 3. X-Ray Diffraction – Burned 2 hr at 700°C.

D - Washed:

As the first step an amount of 100gr potassium hydroxide (KOH) is solved in 250mililitter distilled water. After cooling and reaching ambient temperature, its velocity would be increased to 1Litter, adding ethanol. The resulting solution KOH is a cleaning solution and highly corrosive. In this section, the sample is washed in the KOH solution. Reviewing XRD spectra of the samples (Diagram 4) we'd realize that:

* The intensity of the resulting peaks has greatly lowered. In other words, the process of formation has slowed

* Only SiC phase is restored. In other words, only SiC is formed after washing. And phases of Si and CNT are removed which means that a pure SiC could be produced this way.

*** With Si, being removed, we can conclude that the efficiency in trapping solar energy increases.

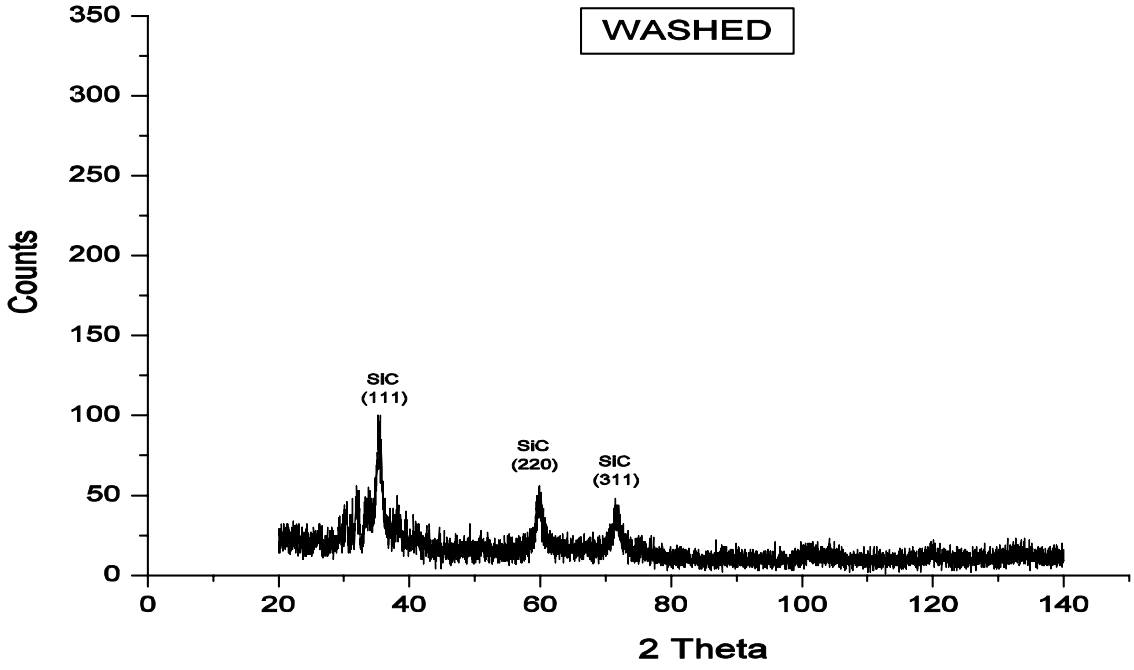

Figure 4. X-Ray Diffraction – Washed in KOH.

Results and discussion

From XRD spectrum, this could be concluded that as the temperature increases, the resulting peaks intensity weakens. Si peak has started to grow from 900° C and is higher at1000° C. With mixture of Si and C we'd come to this conclusion that, at lower temperatures the biggest proportion of Si phase is restored. By sintering Si and C, in addition to restoring Si and CNT, silicon carbide is also restored. By burning the sample, Si and SiC formation rate increases. Only SiC is formed after washing. And phases of Si and CNT are removed which means that a pure SiC could be produced this

way.

SiC emission occurs at wavelength area of 11.3μm or at wave number area of 884.95cm^{-1}. Comparing the spectra of $K = \lambda^{-1} = 825.48$ cm^{-1}, formation of Si-C bond could be seen which is because, the bonding of carbon atoms in acetic acid and ethanol, with the Si bond in hydrolyzed and condensate Tetraethyl orthosilicate liquid ($SiC_8H_{20}O_4$). Also comparing the spectra, we can conclude that, as the temperature increases, the amount of absorption due to SiC, increases as well.

Reviewing the nature of SiC annealed samples in different states, we'll come to the following conclusions:

A - In the case Si and C are mixed, we realized that at low temperatures, the Si phases are mostly restored. However, at this temperature, CNT or carbon nano-tubes will also be restored. These nano-tubes are highly efficient in trapping solar energy, as solar collectors and transmitter.

B - Or in the case of Sintered Si and C we find that in addition to restoring Si and CNT, silicon carbide is also restored. But as their height reduces, their width is decreased. According to Debye – Scherrer equation particle sizes are larger. The reduction in resulting peak intensity indicates the rapid weakening of Si, CNT due to the existing porosity at 1200 ° C.

C -In Burned state, by burning the sample for 2 hours at 700 ° C, we'll realize that the CNT phase is removed and only the Si and SiC phases are restored. In other words, the performance of solar energy trapping has decreased. However, the intensity of Si and SiC peak formation is increased. In other Words by burning samples, Si and SiC formation rate have increased. Due to the peak height increase, the particles tend to form nano-structure particles.

D -In Washed phase, we found that the intensity of the peaks has greatly lowered. Only SiC phase is restored. The pure SiC could be obtained this way. As Si is removed, we may realize that the efficiency of solar energy trapping has increased.

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