International Journal of Academic and Applied Research (IJAAR)
ISSN: 2643-9603
Vol. 6 Issue 6, June - 2022, Pages: 72-77

Synthesis Silicon Dioxide (SiO_2) at Different Temperatures and Study their Optical and Structural Properties

Fawaz Taha Omer*[1], Mubarak DirarAbd Allah[2], Abdalskhi.S.M.H[3], Sawsan Ahmed Elhouri Ahmed[4] & Suliman Alamin AbdElmagid[5]

[1] University of kassala, Faculty of Education Halfa Aljadedah, Department of Physic. [2]International University of Africa, Khartoum-Sudan and Sudan University of Science &Technology-College of Science-Department of Physics-Khartoum-Sudan
[3]AlNeenlen University, Faculty of Science and Technology- Physics Department, Khartoum, Sudan
[4]University of Bahri- College of Applied & Industrial Sciences Department of Physics-Khartoum-Sudan
[5]Kordofan University – Faculty of Science -Department of physics- Kordofan-Sudan

Abstract: *Five samples of Silicon Dioxide (SiO_2) were Synthesed at different temperatures (300,350,400,450 and 500)^OC using hydrothermal method. Structural Characterization , vibritional freqinces and some optical properties were determined using X-ray diffractometer (XRD), Fourier Transform Infrared Spectrophotometer(FTIR) and UV-VIS min 1240 spectrophotometer respectively. All peaks determine transformation of dried powder to SiO_2 crystallites with cubic rutile crystal structure, the grains size of SiO_2 increased from 24.1nm to 55.1nm as the temperature increase from 300^OC to 500 ^OC. For all samples the band positions are present study the absorption bands v_1, v_2, v_3, v_4, v_5, v_6 and v_7 are found to be around455.5 cm^{-1}, 613.4 cm^{-1}, 1027.1 cm^{-1}, 1381.45 cm^{-1}, 2357.09 $cm^{-1}$and 3422.53 cm^{-1} respectively for all the compositions. All optical properties studied in range of (400 - 800) nm wavelength range for SiO_2 samples, the absorption increase from 0.46 (a.u) to 0.64 (a.u) at wavelengths 515 nm as the temperature increase from 300^OC to 500^OC. The maximum reflection observed at wavelength 475 nm equal 0.204 (a.u) then it decreases to zero at wavelength >790 nm, the value of absorption coefficient coefficient increase from 2.1×10^4 cm^{-1} to $2.9\times10^4 cm^{-1}$ at wavelength 515nm as the annelaing temperater increase, finally, the optical energy band gap was decreased from (1.976) eV to (1.937) eV as the temperature increase from 300^OC to 500^OC .*

Keywords*: Silicon Oxide, XRD, FTIR, UV-VIS, grain size and energy gap.*

1. Introduction:

Silicon Dioxide, whose common name is silica, is a white or transparent, crystalline and odorless solid. It belongs to group IV of the chemical family called metal oxides. It is a very stable compound, and only reacts with hydrofluoric acid. Silicon dioxide is an acidic oxide and acidic nature is due to the production of hydrogen ions when it is in water [1]. Silicon dioxide transmits visible and ultraviolet light. Silicon Dioxide comes in many different geometrical patterns [2]. Till date near about 35 crystalline shapes have been observed which results in different density of each group of atoms [3]. SiO_2 is a three-dimensional structure and comes from the tetrahedral structure SiO_4. Each of the Silicon atoms is connected to each other with an oxygen atom, which creates a "diamond type network". The bond angle of Si-O-Si is around 145 degrees [4,5]. Nano-silica particles are divided into P-type and S-type according to their structure. The P-type particles are characterized by numerous nanopores, which have a pore rate of 0.61 ml/g and exhibit a higher ultraviolet reflectivity compared to the S-type; the latter also has a comparatively smaller surface area [6,7]. Silicon dioxide is one of the "building block" for fabrication of semiconductor devices, it can also be an excellent dielectric, it is normally found on a device such as "field oxide" electrically isolating Poly silicon, is also found on the device as a "gate oxide, Silicon dioxide is used in a variety of applications in the electronics and photonics industries, with a corresponding range of desired properties. It can be formed by several methods such as thermal oxidation [9,10]. In this study structural and some optical properties of SiO_2 were studied after annealed at different temperature.

2. Materials and method

In this study extraction and purification SiO_2 were prepared via a hydrothermal method, 150 grams of sand were collected from Kordofan state and then add 100 ml of HCL (7.1 M) to beaker, the acid is transferred to a magnetic stirrer/ hotplate to dissolve the sand's impurities. After heating, the sand will add slowly as CO_2 will be produced according to the equation

$$CaCO_3 + 2HCL \rightarrow CO_2 + H_2O + CaCL_2$$

To condense the acid vapor; boiling ask with ice water is placed on the top of the beaker. The heating will have continued until no more bubbles are produced, after that, the acidic sand will wash with water until become gray in color. The pure sand will transfer to filtered paper for drying. Weight the sand crude SiO_2.80 grams of NaOH put in a stainless-steel crucible, and then 60 grams of the crude SiO_2 were added and mixed will, and Heated until becomes liquid and then stiffens again.

$$2NaOH(l) + SiO_2(s) \rightarrow Na_2SiO_3(s) + H_2O(g)$$

After that quickly remove the mixture from the crucible and put it in a beaker, then added 400 ml of H_2O to dissolve the mixture, Filtrate the mixture using gravity filtration (for 1.5 hours) and Transfer it into glass vessel, and add about 25 ml of 95sulfuric acid drop by drop.

$$2Na(SiO_2) + H_2SO4 \rightarrow 2(SiO_2) + 2Na_2SO_4 + H_2O$$

Filtrate the mixture and wash with water, Excess Silicic acid decomposes to form $SiO_2$and dry it in oven (300, 350,400,450 and 500) ^{O}C for 25 min, finally grind it into fine powder and weight it. X-ray diffraction (XRD), FT-IR spectroscopy and UV-visible spectrometer were carried to find some crystal parameters, vibritional freqinces and some optical properties of SiO_2 samples.

3. Results and Discussion

The crystal structure of all SiO_2 samples characterized at room temperature using a Philips PW1700 X-ray diffractometer (operated at 40 kV and current of 30 mA) and samples were scanned between 30^{O} and 100^{O} at a scanning speed of 0.06 $^{o}C/s$ using Cu Kα radiation with λ = 1.5418Å. The representative XRD charts of all Silicon Dioxide prepared at different temperatures (300,350,400,450 and 500) ^{O}C as show in fig (1)

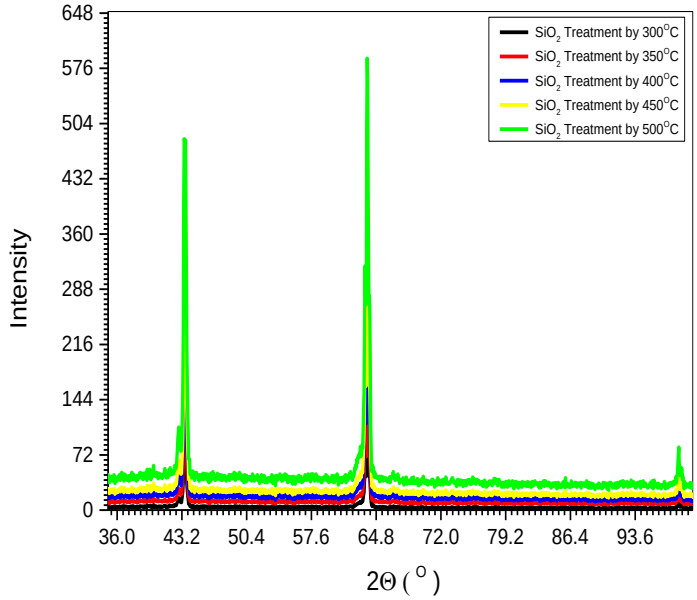


Table (1) crystallite lattice of SiO_2 samples prepared at different temperatures (300,350,400,450 and 500) ^{O}C

Sample	C-form	A=b=c	α=β=γ	Density (mg.cm^{-3})	Xs (nm)	d-spacing 10^{-10} m
SiO_2 Treatment at 300^{O}C	Cubic	81.0	90	0.00011	24.1	1.76845
SiO_2 Treatment at 350^{O}C	Cubic	81.0	90	0.00013	25.1	1.76800
SiO_2 Treatment at 400^{O}C	Cubic	81.0	90	0.00017	46.6	1.3089
SiO_2 Treatment at 450^{O}C	Cubic	81.0	90	0.00019	46.8	1.25052
SiO_2 Treatment at 500^{O}C	Cubic	81.0	90	0.00020	55.5	1.22965

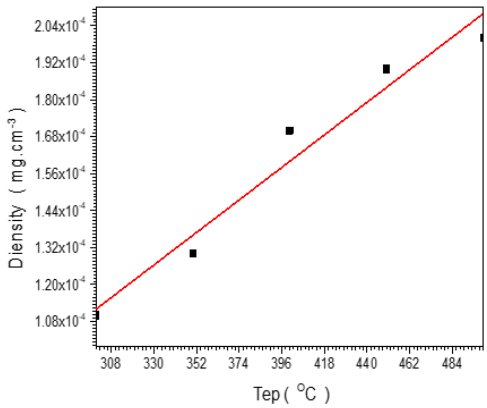


Fig (2) releationship between the density and aneeling temperutare of SiO_2 samples prepared at different temperatures (300,350,400,450 and 500) ^{O}C

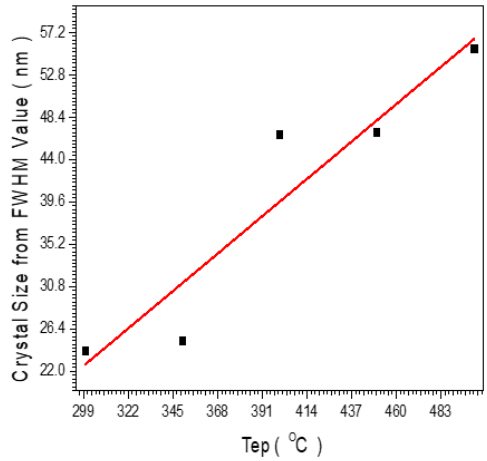


Fig (3) releationship between the Crysllite Size and aneeling temperutare of SiO_2 samples prepared at different temperatures (300,350,400,450 and 500) ^{O}C

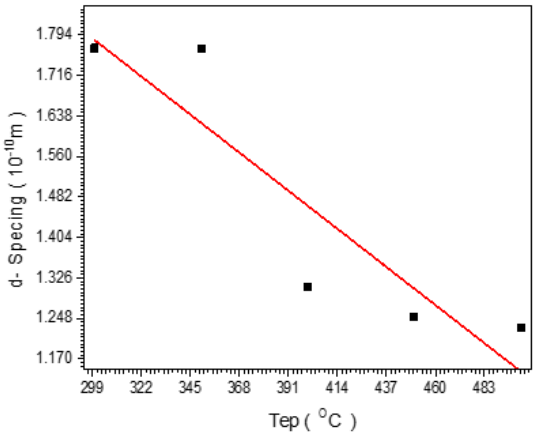


Fig (4) releationship between the d – specing and aneeling temperutare of SiO_2 samples prepared at different temperatures (300,350,400,450 and 500) ^{O}C

Miller indices provided in the figure and all peaks determine transformation of dried powder to SiO_2 crystallites with cubic form. Table (1) shows the XRD parameters of SiO_2 nano powder at various crystalline orientations. It was found that the annealing lead to decrease in d-space from (1.76845 to 1.22965) 10^{-10} m while dislocation density and grains size increase from (0.00011 to 0.00020) mg.cm^{-3} and (24.1 to 55.1) nm respectively and this sue to increase in temperature lead to increase the crystallinity of material. The relationship between annealing temperate and dislocation density, grains size and d-space were shown in figs (2), fig (3) and fig (4) respectively.

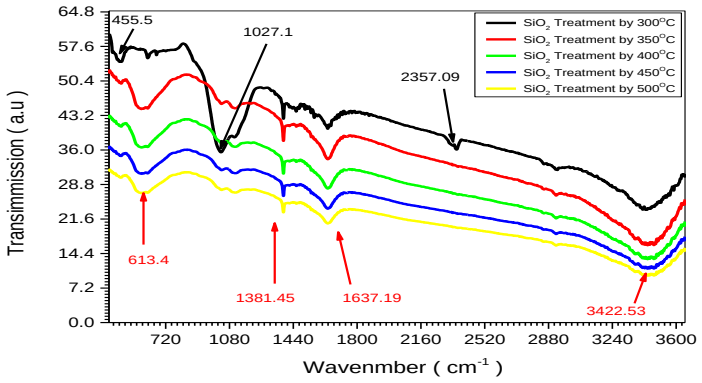


Fig (5) FTIR spectrum of SiO_2 samples prepared at different temperatures (300,350,400,450 and 500) ^{O}C

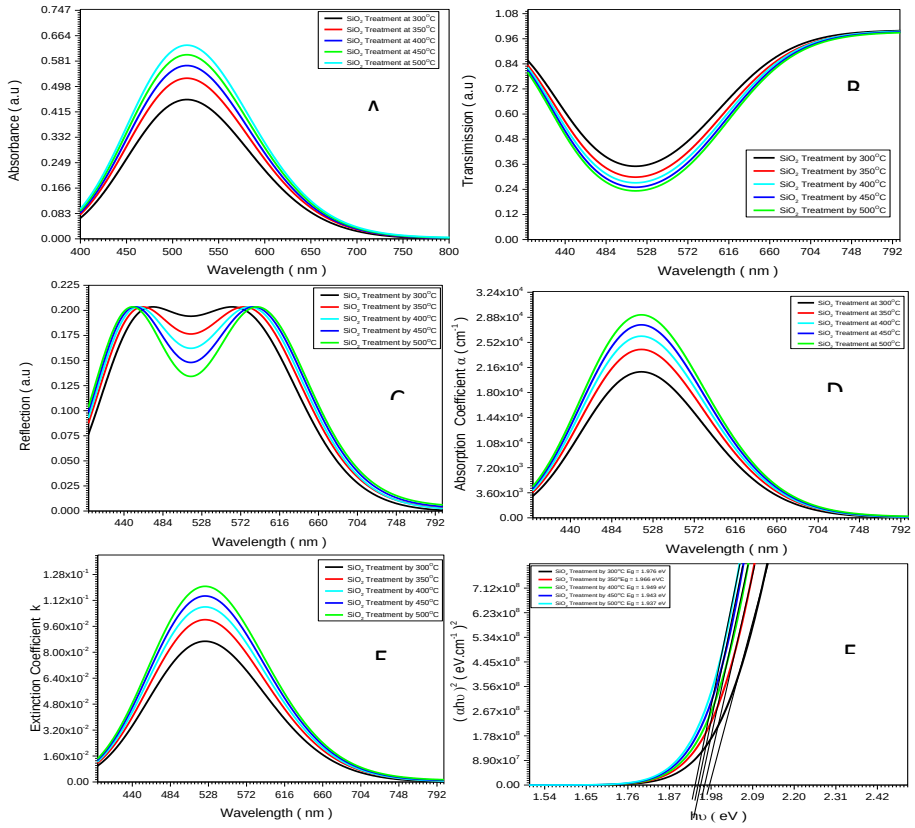
Table (2) Parameters of SiO_2 samples preperaed at different temperatures (300,350,400,450 and 500) ^{O}C

No.	**Compounds**	υ_1	υ_2	υ_3	υ_4	υ_5	υ_6	υ_7
1	SiO_2 Treatment at 300^{O}C	455.5	613.4	1027.1	1381.45	1637.19	2357.09	3422.53
2	SiO_2 Treatment at 350^{O}C	-	613.4	-	1381.45	1637.19	-	3422.53
3	SiO_2 Treatment at 400^{O}C	-	613.4	-	1381.45	1637.19	-	3422.53
4	SiO_2 Treatment at 450^{O}C	-	613.4	-	1381.45	1637.19	-	3422.53
5	SiO_2 Treatment at 500^{O}C	-	613.4	-	1381.45	1637.19	-	3422.53

The infrared spectra of SiO_2 samples synthesized at defferant temperatures aneeling powders(300 ,350 ,400 ,450 and 500)^{O} C were recorded by mattson Fourier Transform Infrared Spectrophotometer in the range of 400 to 3650cm^{-1} which shown in fig(5) . The spectra of all samples have been used to locate the bonds positions which are given in the Table (2), the absorption bands ν_1, ν_2, ν_3, ν_4 , ν_5, ν_6 and ν_7 are found to be around 455.5 $_{cm-1}$, 613.4 cm^{-1}, 1027.1 cm^{-1}, 1381.45 cm^{-1}, 2357.09 cm^{-1}and 3422.53 cm^{-1} respectively for all the compositions. The transmiattance bands within these specific limits reveal the formation of single-phase spinel structure having two sub-lattices tetrahedral (A) site and octahedral (B) site. The (ν_1)and (ν_2) band around 455.5 cm^{-1} and 613.4 cm^{-1} is caused by the metal-oxygen vibration in the tetrahedral sides. This difference in the spectral positions is due to the different values of metal ion-O^{-2} distances for octahedral and tetrahedral sites. The band (ν_3) around 1027.1 cm^{-1} is due to C-C stretch and C-C-H bending. The band (ν_4) around 1381.45 cm^{-1} is associated with the O-H bending vibration. The band (ν_5) around 1637.19 cm^{-1} is due to C=C stretching. (ν_6, ν_7) around 2357.09 cm^{-1}and 3422.53 cm^{-1} is due to the stretching mode of H-O-H bending vibration of free or absorbed water which implies that the hydroxyl groups are retained in ferrites .

UV-VS min 1240 spectrophotometer was used to study the absorbance of SiO_2 samples prepared at different temperatures (300,350,400,450 and 500) ^{O}C and then use it to calculate some optical properties as shown in fig (6). fig(6-A) shows the relation between wavelengths and absorbance of SiO_2 samples , the rapid increase of the a absorption at wavelengths 515 nm from 0.46 (a.u) to 0.64 (a.u) as the temperature increase from 300^{O}C to 500^{O}C. Fig (6-B) show that the transimission is opissite behavior of absorbance, meaning that the sample which have high value of absorbance have low value transmitance. The reflectance (R) of SiO_2

samples prepared at different temperatures spectra in the (400 - 800) nm wavelength range display in fig (6-C). The maximum reflection observed at wavelength 475 nm equal 0.204 (a.u) then it decreases to zero at wavelength >790 nm. The maximum reflection edge of SiO_2 samples occurs at wavelength (475 nm) corresponding to photon energy (2.6 eV). The absorption coefficient (α) of SiO_2 samples prepared at different temperatures were obtained from the following relation $\alpha = \frac{2.303 \times A}{t}$ where (A) is the absorbance and (t) is the optical legth in the samples. From fig (6-D) the absorption coefficient increase from 2.1×10^4 cm^{-1} to $2.9\times10^4 cm^{-1}$ at wavelength 515nm as the annelaing temperater increase in the visable region, this means that the transition must corresponding to a direct electronic transition, and the properties of this state are important since they are responsible for electrical conduction. Also, fig.(6-D) shows that the value of (α) for the five samples of SiO_2 increase while the tempeutoer aneeling increased .Extinction coefficient (K) was calculated using the related $k = \frac{\alpha\lambda}{4\pi}$ The variation of (K) values as a function of (λ) are shown in fig (6-E) ,it is observed that extinction coefficient (K) as the same as absorpton coefficient , it is increase from 8.72×10^{-2} to 1.22×10^{-1} as the temperature increase from increase from 300^OC to 500^OC . The optical energy gap (Eg) has been calculated using Tauc equation $(\alpha h\upsilon)^2 = C(h\upsilon - Eg)$ where (C) is constant. By plotting $(\alpha h\upsilon)2$ vs photon energy ($h\upsilon$) as shown in fig.(6-F) for SiO_2 samples prepared at different temperatures and extrapolating the straight thin portion of the curve to intercept the energy axis which is value of energy gap, the value of(Eg) was decreased from (1.976) eV to (1.937) eV as the temperature increase from 300^OC to 500^OC .



Fig(6) Some optical properties of SiO_2 samples prepared at different temperatures (300,350,400,450 and 500) ^OC

4.Conclusion

Silicon dioxide (SiO_2) nanoparticels have been successfully synthesized at different temperatures (300,350,400,450 and 500) ^OC. As the properties of the obtained material, it can be used in optoelectronic application such as solar cell, gas sensor,chemical sensors and electronic chips.

References

[1] Tari, F.; Shekarriz, M.; Zarrinpashne, S.; Ruzbehani, A. Catalytic and environmentally friendly removal of hydrogen sulfide from Claus-derived molten sulfur by nanosilica. Int. J. Environ. Sci. Technol. 2019, 16, 1691–1700.

[2]Violeta Purcar and et al , Preparation and Characterization of Silica Nanoparticles and of Silica-Gentamicin Nanostructured Solution Obtained by Microwave-Assisted Synthesis, Materials, MDPI, Materials 2021, 14, 2086.

[3] Wooldridge, M.S.; Torek, P.V.; Donovan, M.T.; Hall, D.L.; Miller, T.A.; Palmer, T.R.; Schrock, C.R. An experimental investigation of gas-phase combustion synthesis of SiO2 nanoparticles using a multi-element diffusion flame burner. Combust. Flame 2020, 131, 98–109.

[4] Devi, M.G.; Balachandran, S. A Review on synthesis, characterization and applications of silica particles. Int. J. Eng. Res. Technol. 2016, 4, 249–255.

[5] Biomass derived silica containing products for removal of microorganisms from water. Int. J. Environ. Sci. Technol. 2015, 12, 1495–1502.

[6] Nora H. Mutesher and Firas Jawad Kadhim, Comparative Study of Structural and Optical Properties of SiO_2 Nanoparticles Prepared by DC Reactive Sputtering and Sol-Gel Route,

[7] Mohammed A. Hameed, Zahraa M. Jabbar, "Preparation and Characterization of Silicon Dioxide Nanostructures by DC Reactive Closed-Field Unbalanced Magnetron Sputtering" Iraqi Journal of Applied Physics, 5, 2016.
[8] Hayder G. Fahad, Oday A. Hammadi, "Characterization of Highly-Pure Silicon Dioxide Nanoparticles as Scattering Centers for Random Gain Media" Iraqi Journal of Applied Physics, 16, 2020.
[9] Gounani, Z.; Asadollahi, M.A.; Meyer, R.L.; Arpanaei, A. Loading of polymyxin B onto anionic mesoporous silica nanoparticles retains antibacterial activity and enhances biocompatibility. Int. J. Pharm. 2018, 537, 148–161.
[10] Basu, H.; Singhal, R.K.; Pimple, M.V. Reddy AVRR Synthesis and characterization of silica microsphere and their application in removal of uranium and thorium from water. Int. J. Environ. Sci. Technol. 2015, 12, 1899–1906.