ESTONIAN UNIVERSITY OF LIFE SCIENCES
Institute of Technology

Indrek Alberg

ABSORPTION SPECTROSCOPY STUDIES OF SILICON DIOXIDE NANOPARTICLES AND THEIR APPLICATIONS IN SOLAR CELLS

RÄNIDIOKSIIDI NANOOSAKESED JA NENDE RAKENDUS PÄIKESEPANEELIDES

Bakalaureusetöö
Tehnika ja tehnoloogia õppekava

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Käesoleva töö eesmärk on analüüsida erinevaid sool-geel meetodil Eesti Maaülikooli Tehnikainstituudis sünteesitud ränidioksiidide proove UV-Vis spektromeetri abil. Ränidioksiid (SiO_2) on keemiliste elementide räni (Si) ja hapniku (O_2) kombinatsioon. See on Maal väga laialt levinud materjal peamiselt kvartsi ja liiva kujul. Ränidioksiidi kasutatakse dopeeritud pooljuhtelement räniplaatide katmiseks päikesepaneelide fotogalvaanilistel elementidel. See väldib pooljuhtelemendi räni oksüdeerumist ning ühtlasi kaitseb seda väliskeskkonna mõjude eest. Samuti kasutatakse ränidioksiidi valguse peegeldumise vähendamiseks või siis soovitud peegeldumise saavutamiseks kombinatsioonis ainetega, millel on erinev refraktsiooniindeks. Puhta amorfse pooljuhtelemendi ränipinna passiveerimine võimaldab säilitada, tõsta fotogalvaanilise elemendi kasutegurit ning vähendada võimalikke kadusid. Tsooniteooria kohaselt on ränidioksiidi keelutsoon lai. SiO_2 keelutsooni energia (valentsitsooni ja juhtivustsooni vahe) on vahemikus 7,52 kuni 9,6 eV (elektronvolt), mis sõltub Si-O-Si sidemenurgast ja pikkustest. Iga SiO_2 proovi jaoks tehti lihtsustatud arvutused, kasutades Beer-Lamberti seadust. UV-Vis spektromeetri abil saadud tulemusi analüüsiti tarkvaras nimega “Origin” ja joonestati neeldumisgraafikud. Läbiviidud proovide analüüsi tulemused võivad aidata neid SiO_2 proove paremini mõista.

Märksõnad: Ränidioksiidi nanoosakesed, UV- neeldumine, UV- spektroskoopia.

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Silicon dioxide, or silica (SiO_2) is a combination of chemical elements silicon (Si) and oxygen (O_2). It is a very widespread material on Earth mainly in form of quartz and silica sand. Silicon dioxide is used in silicon solar cells on pure silicon wafers for surface passivation and antireflection. Surface passivation is a technique for preventing efficiency losses. Silicon dioxide has a bandgap energy from 7.52 to 9.6 eV (electron volt) depending on Si-O-Si bond angle and lengths. The aim of this Bachelor´s thesis is to analyse four different SiO_2 nanoparticle samples synthesized at the Institute of Technology under UV-Vis spectrophotometer in order to find most UV and daylight absorption. The simplified model based on Beer-Lambert law was implemented to describe absorption in these silicon dioxide nanoparticle suspensions. As a result, the optical properties of these silicon dioxide nanoparticles were analysed in software named "Origin" and graphs interpreted. Conducted tests results may help to understand these SiO_2 samples more.

Keywords: SiO_2 nanoparticles, UV-Vis absorption, UV-Vis spectroscopy.

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INTRODUCTION

The rapid increase in the population, industrialization and modern life standards has resulted in the depletion of energy sources, which has pushed the scientific community to develop a more green and sustainable approach for energy production. In this regard, Solar and wind parks are an emerging and alternative way for greener energy production in comparison with the traditional technologies. Solar cells are usually made up of materials like pure silicon, silicon dioxide, copper, cadmium, gallium and shows an efficiency of 15-20% which is not enough to meet the current energy demands. Therefore, researchers are investigating different materials and their combinations to increase the efficiency of solar cells. The efficiency of the current solar cell panels is around 15-20% which is not sufficient for their large-scale implementation. In fact, the purity of the materials used in solar cells, energy losses in the form of heat and photovoltaic element degradation critically affect the efficiency of a solar cell. Nanomaterials with at least one characteristic dimension in the range of 1 to 100 nm carry some unique properties that have shown their potential in various fields of engineering and medical sciences. However, they can serve as a suitable material for the development of solar cells exhibiting higher efficiency in comparison with traditionally used materials. In fact, nanomaterials can create a solar cell with a thin and large surface area resulting in the reduction of material use and overall cost of the solar cell.

In this thesis, I have investigated the absorption behaviour of the SiO_2 nanoparticles synthesized in the Nanotechnology and materials sciences laboratory at the Institute of Technology. The work includes studying the absorption spectrum and analysing adsorption peaks of different SiO_2 samples using a UV-Vis spectrophotometer. The adsorption studies will help us to find and determine their absorption quality to have feedback for possibly applying them to the next generation of photovoltaic cells.

1. REVIEW OF LITERATURE

1.1. Solar Panel and Solar cells

A solar panel is designed to absorb sun rays as the main source of energy for producing current or heating. It consists of different layers (Figure 1) corresponding to its overall working performance and efficiency.

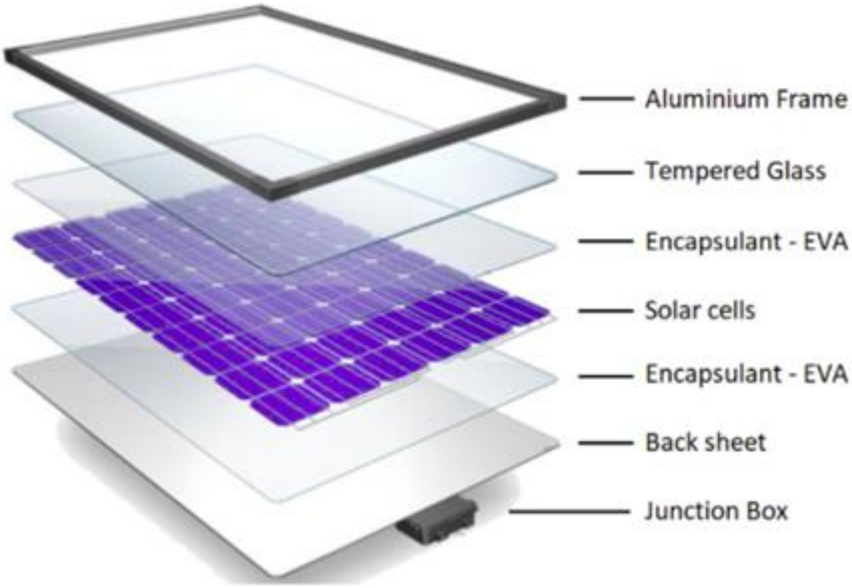


Figure 1. A typical Solar panel along with its different layers. [1]

The workability and effectiveness of a solar panel are dependent on the efficiency of solar cells inserted in between the layers of ethylene-vinyl acetate (EVA). EVA contributes to the safety, insulation, sound insulation, and anti-ultraviolet barrier in the panel. Solar cells are devices with the capability to convert light energy into electrical energy. They are more particularly applied in powering space equipment i.e. Hubble telescope and in addition, they offer a cost-effective approach to power various electrical devices. Therefore, they are getting more and more attention in the scientific community. Despite their notable advantages, their shortcomings cannot be ignored. For example, solar cells are weather dependent which affects their efficiency on rainy or cloudy days and in winter with shorter days, uses a lot of space, and their storage is quite expensive which put a significant effect on their applicability at a large scale. To overcome such drawbacks, extensive and in-depth research to increase the working efficiency of solar cells is still required [1]. A typical solar cell is made up of different components (Figure 2) which contributes to their overall working efficiency.

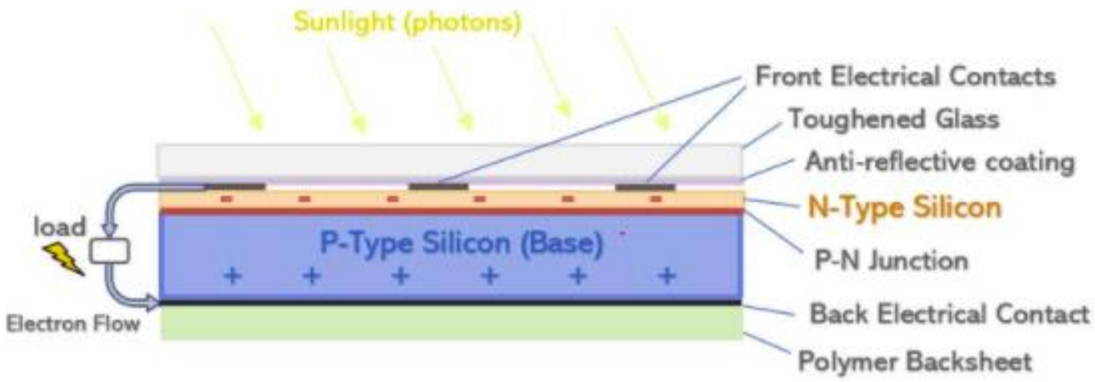
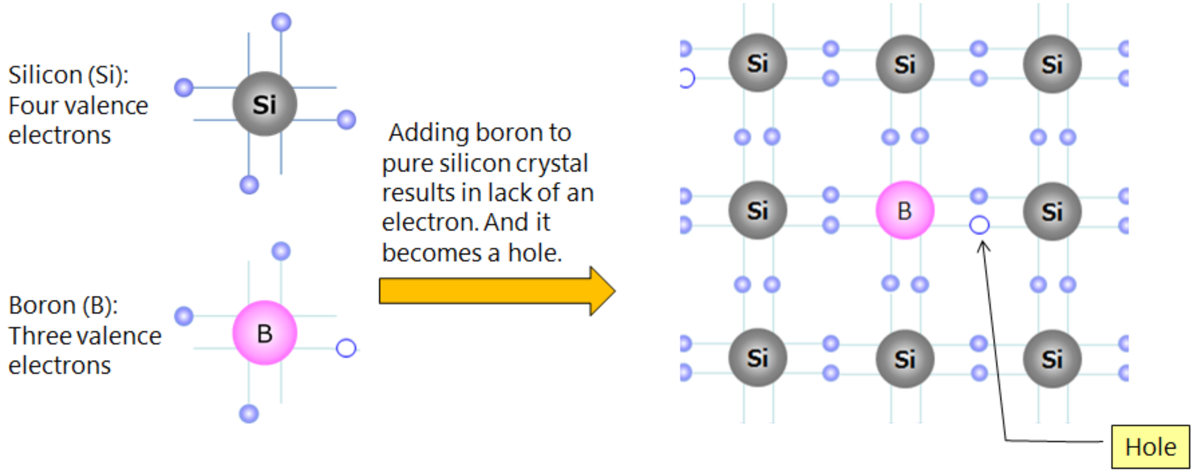


Figure 2. Solar cell construction. [1]

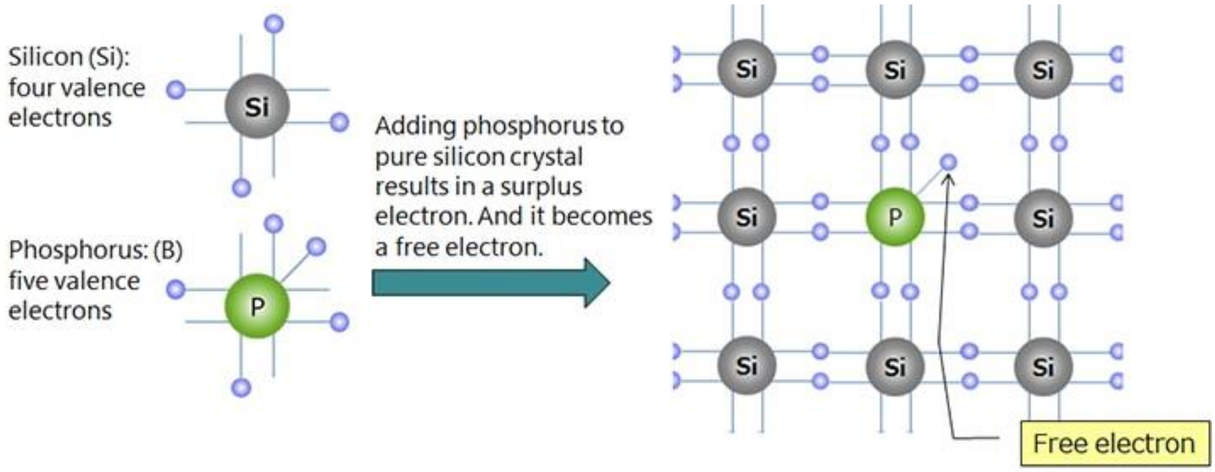
When a particular wavelength of light falls on the surface of a material, it triggers the migration of electrons from a ground state to some excited state resulting in the formation of free electrons and holes. This phenomenon is generally referred to as the photovoltaic effect. This effect produces a voltage or electric current. Conventional crystalline silicon (c-Si) solar cell when doped with various chemical elements i.e. Boron and Phosphorous enhances its power production and are more abundantly utilized in designing solar cells. Basically, solar cells are made up of two different types of semiconductors: a P-type and an N-type. The P-type semiconductor is a boron-doped semiconductor that has one less electron compared to silicon. The P-type semiconductor having the deficiency of electrons is thus a positively charged entity which is represented as a hole (Figure 3).



Adding boron to pure silicon crystal results in lack of an electron. And it becomes a hole.

Figure 3. P-type semiconductor. [2]

Whereas, an N-type semiconductor is doped with Group V chemical element like phosphorus (P) to incur an impurity (see figure 4) [2]. The phosphorous doped silicon has one extra electron than silicon which is free to move around and contributes to the current generation.



Adding phosphorus to pure silicon crystal results in a surplus electron. And it becomes a free electron.

Figure 4. N-type semiconductor. [2]

The combination of these semiconductors is usually named as a p-n junction. The excess holes and electrons in the P-type and N-type results in the generation of a potential difference and the electric field created by the space charge region oppose the diffusion process for both electrons and holes [3]. This electric field affects negatively charged particles to move in one direction and positively charged particles in the other direction. With a particular wavelength of light, energy from the photon is transferred to an electron of the semiconducting material, causing its excitation to an advanced energy state named the conduction band [4]. The electrons present in the conduction band are free to move around and thus contributes to the current generation. The main objective behind making photovoltaic devices corresponds to their reducing cost, improving conversion efficiency, and the ability to substitute traditional fossil energies.

1.2. Nanomaterials: Applications and characterization

Nanomaterials (NM) at a size less than 100nm is considered as nanoscale which exhibits some notable properties such as high surface area, porosity, specific surface charge, surface functionality, and ions binding capabilities that cannot be observed in bulk materials. Due to these qualities, the concept of nanotechnology or nanoparticles (NPs) is used in solar cells manufacturing as it reduces manufacturing costs. Moreover, because of low-temperature processing in comparison to typically used processes to produce conventional semiconductors based cells, nanomaterials serve as a way to make more efficient materials in order to design sustainable and more effective solar cells. These nanoparticles can also reduce the installation costs of solar cells due to their unique characteristics. Currently, available nanotechnology solar cells are not as efficient as traditional ones, but researchers investigate how to improve the efficiency using quantum dots [5].

Solar cells can be classified into three generation technologies. The first-generation solar cell silicon wafers are estimated to have a power conversion efficiency approx. 25.6%. Whereas, the second-generation solar cells are thin films and were fabricated with amorphous silicon, CdTe or copper indium gallium diselenide (CIGD) and have exhibited an efficiency of approx. 19.6%. Third-generation solar cells are nanomaterials-based solar cells, these include dye-sensitized solar cells (DSSCs), quantum dot, hybrid, organic and perovskite solar cells (named PSCs). DSSCs and PSCs are unique due to their performance in the research field of photovoltaic and can approach the radiative efficiency limit (~33,7%) [6]. Silicon is the most abundant element on Earth and is mostly used in PV devices. Various modifications like creating defects in the crystal structure are being widely researched and investigated during recent years.

Nanoparticles exhibit some unique optical properties that are dependent on their shape, size, concentration, agglomeration, and refractive index on their surface. UV-Vis spectroscopy is mostly used for determining analyte concentrations or the chemical conversion of a component in a solution. This makes UV-Vis a valuable tool for classifying, describing, and studying different nanomaterials [7]. Silica nanoparticles have been implemented in high-tech applications for their good physicochemical, mechanical and optical properties. Silica is very abundant on Earth (sand) making it cheap and can be easily extracted.

1.3. Silica nanoparticle: Optical Properties and their applications

Silica nanoparticles are being widely studied for their potential as photonic crystals, chemical sensors, biosensors, nanofillers for composite materials, markers for bioimaging, as substrate for quantum dots and catalysts [8]. Additionally, optical absorption and emission properties, specific surface area and density are also important parameters. Silicon solar cells (SC) shows a great response in the spectral range from 500 to 1000 nm. The redshift of the short wavelengths offers a rise in the energy conversion efficiency of the silicon SC with no substantial increase in the manufacture cost [9]. Several studies on silicon dioxide nanoparticles were performed. For instance, Attafi et al. investigated the enhancement of silicon solar cell performance by introducing selected defects in the SiO_2 passivation layer. It was found that the integration of selected defects in the silicon oxide region of a silicon solar cell increases its efficiency. Defects on the front and back surface of silicon (Si)–based solar cell can be passivated by depositing an additional layer of silicon oxide (SiOx) [10]. They did several simulations with n-type silicon-based solar cell (as shown in Figure 5) together with deep level defects in the silicon dioxide (SiO_2) passivation layer [10].

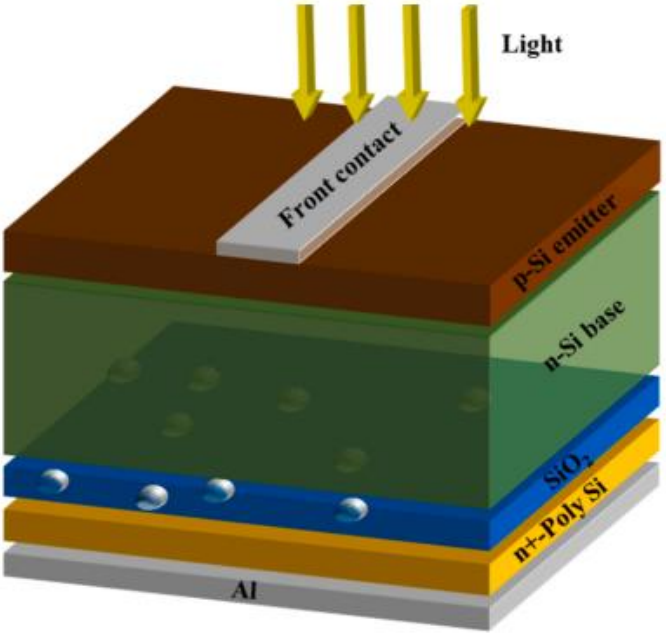


Figure 5. Schematic view of the simulated pnn$^+$ silicon solar cell. SiO_2 is the passivation layer. [10]

Nano-SiO_2 is the most used among widespread inorganic nanoparticle. For example, by adding nano-SiO_2 into the coating formation, the mechanical, thermal, weather resistance and anti-corrosion properties of the organically manufactured coatings are significantly improved [11]. Nano-SiO_2 is also used for superhydrophobic and hydrophilic coatings, for example in car clear coatings, which can create better abrasion resistance. Nguyen et al. studied the effects of nano-SiO_2 on improving the weathering resistance in polyurethane coatings. There were 3 altered polymer samples produced in a laboratory. The study showed that incorporation of nano-SiO_2 in the acrylic polyurethane matrix improved its mechanical properties and also enriched its weathering resistance [11]. This study showed that UV absorption of nanofillers (nano-SiO_2) could protect the polymer coating. Characterizations of absorption and scattering in nanoparticles were examined in a study by Wang et al. They carried out a spectrophotometry study on different dimension silicon-dioxide nanoparticles. Figure 6 shows the UV–Vis spectra of nanoparticles with a diameter of 50 nm – 200 nm of non-metallic oxides like silicon dioxide (SiO_2) [12].

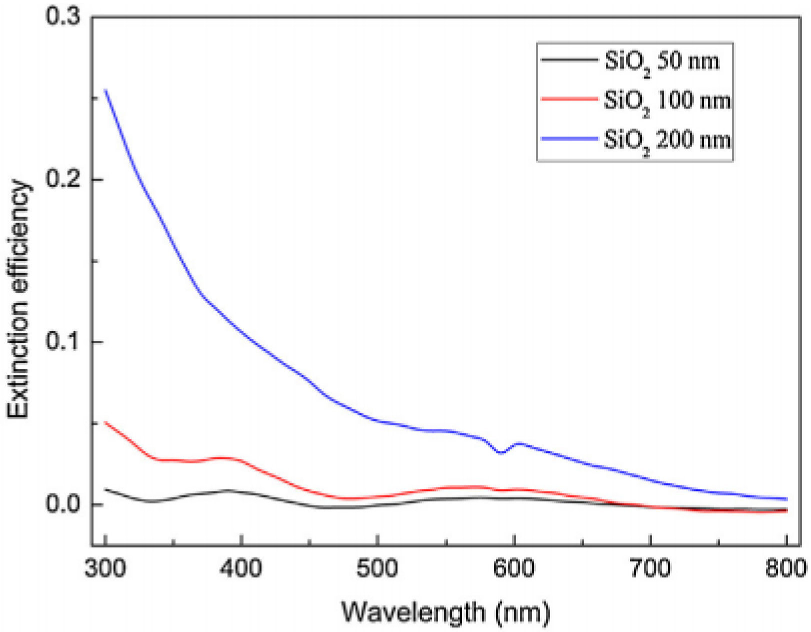
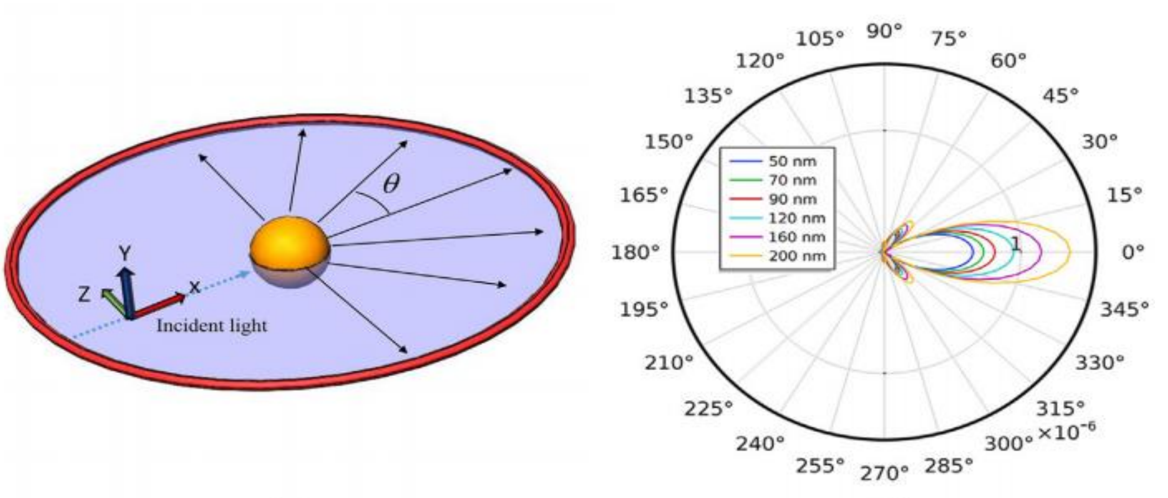


Figure 6. UV–Vis spectra of SiO_2 nanoparticles with different sizes. [12]

This study concluded that the optical properties of nanoparticles are size dependent [12]. In the visible light (400-700 nm) nanoparticle extinction (absorption) efficiencies are size dependent.

In a study by Wang et al the scattering of different size SiO_2 nanoparticles was also examined. Far-field scattering is a light emission in the far field region. Far-field scattering by nanoparticles can be interpreted by using polar diagrams. The schematic diagram of far-field scattering by nanoparticles and the polar diagram of scattering of SiO_2 nanoparticles with different sizes are displayed in Figure 7.



(a) (b)

Figure 7. (a) Graphic describing the far-field scattering of nanoparticles. (b) The polar diagram of the scattering of SiO_2 nanoparticles with different sizes. [12]

The angle between the scattering light and the x-axis was marked as θ. Different size SiO_2 nanoparticles scattered weakly at small angles and scattered more in big angles as shown in Figure 7. (b) [12].

Attafi et al. investigated the enhancement of silicon solar cell performance and it was found that a combination of the SiO_2 layer and the heavily doped poly-Si attains excellent surface passivation properties and preserves, excellent contact resistance properties at the same time [10]. The solar cell performance was simulated with the presence of defect levels inside the SiO_2 bandgap as shown in Figure 8.

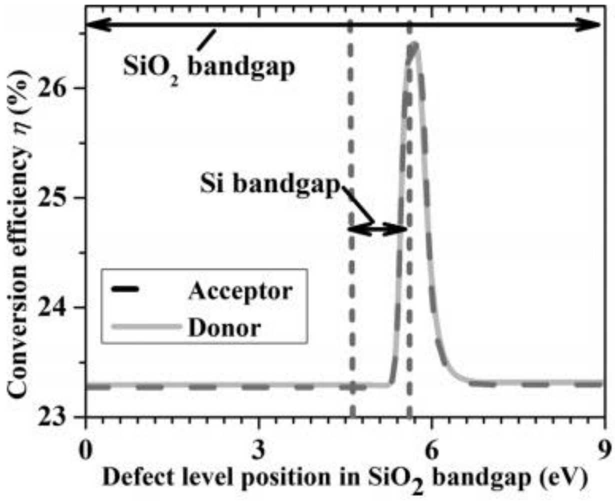


Figure 8. The solar cell efficiency (η) evolution as a function of the defect level position. [10]

The altered solar cell efficiency η reached 26 %. Acceptor and donor deep levels were slightly above the silicon conduction band minimum (CBM) [10]. It was concluded that the incorporation of selected defects in the SiO_2 passivation layer can enhance the solar cell efficiency of both n-type and p-type Si-based solar cells [10].

Surface passivation in Si-based solar cells is a process where the semiconductor (Si) surface is transformed inert thus reducing the probability of oxidisation. Insulating the semiconductor (Si) with SiO_2 layer enables electricity to reliably penetrate to the semiconductor (Si). This helps to reduce some losses in silicon-based solar cells. Also, SiO_2 can protect and prevent premature deterioration of the electrical characteristics of p–n junctions. One of the most applied surface passivation is thermally grown SiO_2. Thus the approach is to lower the temperatures for thermal growing to achieve more production efficiency. The potential to achieve better efficiency solar cell is higher when surface passivation is applied on the front and rear surfaces of the cell. The key element is to reduce carrier recombination and also to increase internal reflection by trapping light within the solar cell. This makes possible photons bounce back and thus have more probability to excite electrons of the doped semiconducting material (Si). The electrons present in the conduction band are free to move around and to recontribute to the current generation. Besides surface passivation application SiO_2 helps to reduce potential-induced degradation and to protect the semiconductor charge carrier (Si).

2. AIMS OF THE STUDY

The main aim of my study was to characterize the sol-gel synthesized silicon dioxide samples using a UV-Vis spectrophotometer.

However, the main aim consists of various sub-steps:

1. Preparation of different concentrations of SiO_2 samples
2. Characterization through UV-Vis spectrophotometer;
3. Analysis of the absorption peaks.

Through this study, we will have a better understanding of the absorption bands of SiO_2 nanomaterials and the implementation of these nanomaterials in improving the effectiveness and efficiency of solar cells.

3. MATERIALS and METHODS

3.1. Materials and Chemicals

For the experiments chemicals i.e., Isopropanol, silicon dioxide were purchased from Alfa-Aesar and materials i.e., beakers (100mL), mortar-pestle, cuvettes were used to measure the absorbance. All the solutions were prepared using isopropanol as a solvent.

3.2. Analytical technique

3.2.1. Spectrophotometry

Spectrophotometry is a method to measure the amount of light absorbed by a chemical substance based on the intensity of incident light that passed through a sample (see figure 9). It is one of the most useful and widely used quantitative analysis method in different scientific fields such as physics, chemistry, material sciences and medicine.

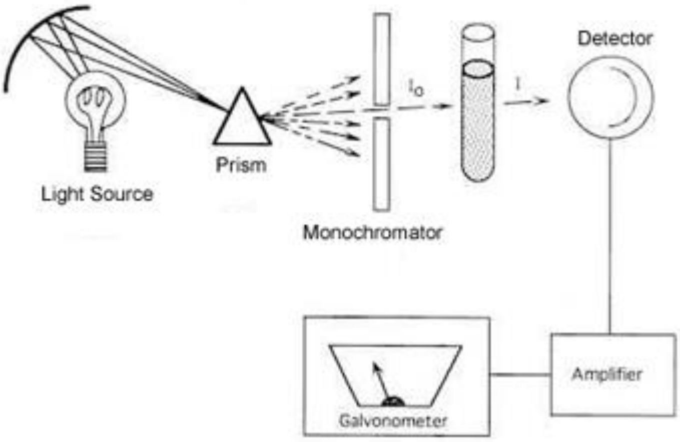


Figure 9. Schematic of a spectrophotometer. [13]

Any chemical substance absorbs, transmits, reflects and scatter light over a certain range of wavelength. A spectrophotometer is an instrument that can measure the intensity of light absorbed by the sample and can quantify the amount of the chemical substances by measuring the intensity of light detected. Based on the wavelength range, it can be classified into UV-Vis (185-700nm) and IR (700-15000nm) spectrophotometer. Generally, IR spectroscopy is used to identify the different functional groups present in a molecule whereas UV-vis spectroscopy is a much more quantitative technique. Therefore, for this study, we have used UV-Vis spectrophotometry to characterize and analyse the adsorption peaks.

3.2.2. UV-Vis spectrophotometer

A UV-Vis spectrophotometer measures the difference in the intensity of light passing through a sample (poured in a cuvette), and the intensity of the incident light. The main components of a UV-Vis spectrophotometer include a light source, sample holder (cuvette), a dispersive device to separate the different wavelengths of the light (e.g. a monochromator), and a suitable detector. The detector in a UV-Vis spectrometer measures the intensity of light that has passed through the sample solution. This fraction of light collected by the detector is named the transmitted intensity, I. The intensity of the transmitted light is enervated when passed through the sample and its value is lower than the original intensity I_0 at the light source. Transmittance can be explained as an equation [14]:

$$\mathrm{T} = \frac{I}{I_0} \tag{1.1}$$

In particular, the UV-Vis spectrophotometer determines the transmittance values but additionally, it can also record the absorbance values which is represented mathematically as the negative of the logarithm of the transmittance and is considered as a unitless value.

$$\mathrm{A} = -\log(T) \tag{1.2}$$

In general, a UV-Vis spectrum is graphically represented as absorbance as a function of wavelength (see figure 10) and the height of the absorption peaks directly indicates the concentrations of the concerned elements. A higher concentrated sample solution will absorb more light and thus shows an increase in the height of the absorption peak (see figure 11). In addition, the attenuation is also proportional to the length of the cuvette; a longer cuvette will lead to higher absorption of light.

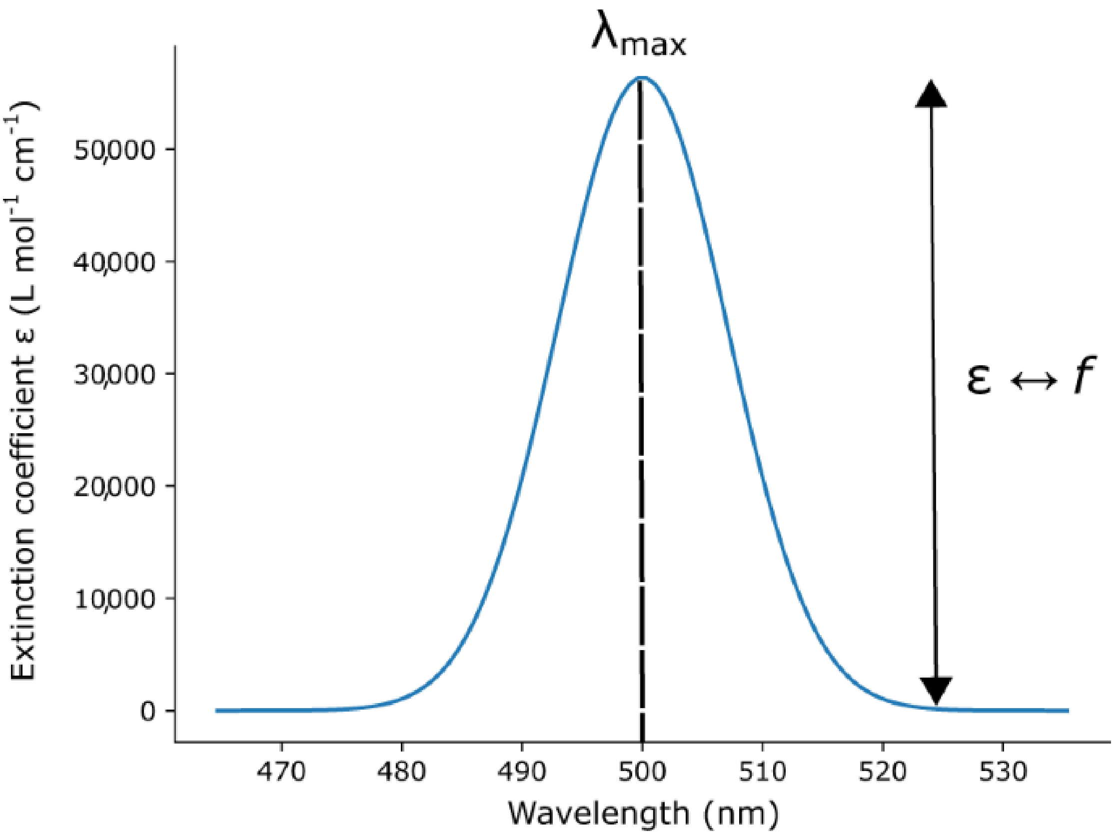


Figure 10. A general UV-Vis absorbance spectrum. [15]

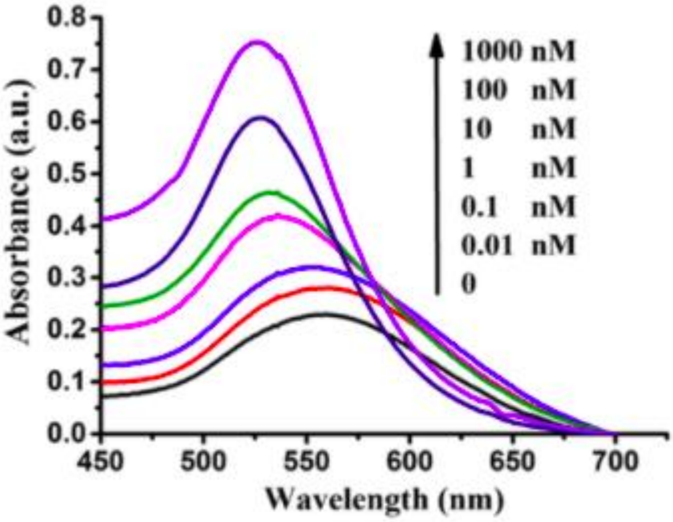


Figure 11. A UV-Vis absorbance spectrum at different concentrations. [16]

The UV spectrum shows variously defined peaks corresponding to a particular chemical entity either pure or decomposed. The maximum absorbance values are represented as λ_{max}. Through this spectrum, we can determine the extinction coefficient of the sample, rate of reaction, and melting point of biological molecules i.e. proteins.

3.2.3. The Beer-Lambert law

The Beer-Lambert law states that there is a linear relationship between the concentration and the absorbance of the solution, which makes possible the concentration of a solution to be calculated by measuring its absorbance [14]. Lambert's law of absorption states that equal parts in the same absorbing medium absorb equal fractions of the light that will enter them [17]. Beer’s law also applies and states that the fractional loss of power due to absorption when an infinitesimal increase is made in the concentration is proportional to that infinitesimal increase [17]. It can be said that the Beer-Lambert law never fails if monochromatic light is used and if the concentration factor in the law is the concentration of the absorbing species (sample) [17].

The Beer-Lambert law has been explained in a form of equation [17]:

$$\mathrm{A} = -log10 \cdot \frac{P}{P0} = a \cdot b \cdot c, \qquad (1.3)$$

where A is the absorbance, formerly called the optical density, without unit;
P is radiant power, formerly called the intensity;
a is molar absorptivity (probability of electronic transition), formerly called the extinction coefficient, ($M^{-1}cm^{-1}$);
b is the length of the beam in the absorbing sample, cm;
c is the concentration of the absorbing sample, (M). [17]

Beer-Lambert´s law is a well-defined method to characterize a variety of materials through their absorption behaviour.

The transmittance and absorbance are inversely related. This means, the more a particular wavelength of light is absorbed by a substance, the less it is transmitted.

3.3. Preparation of the samples

Four different silicon dioxide samples were studied, synthesized by sol-gel routes. To measure their absorbance spectrum, the samples were passed through a UV-Vis spectrophotometer having a wavelength ranging from 190-1100 nm. The samples were prepared by the applying next steps:

1. Crushing the sample using mortar and pestle to make it a homogenous fine powder.
2. Weighing a defined amount of the sample by an analytical weighing balance.
3. Dissolving the weighed samples in isopropanol to make a solution of defined concentration.
4. The absorbance of all the samples was measured and the blank solution measure (isopropanol) was automatically subtracted from the sample measurement.

It is very important to prepare a homogenized solution for all the samples. The nanoparticles were uniformly dispersed in the solvent upon ultrasonic bath (Figure 12).

Figure 12. Dissolution of our sample using a sonicator.

The solution concentration (Ci) was calculated by using the formula:

$$\text{Ci} = \frac{sample\ weight}{solvent\ weight} * factor\ for\ 1\ litre \qquad (1.3)$$

The solution molarity was calculated by using the formula:

$$C(SiO_2)=(\text{sample weight})/(\text{molar mass of } SiO_2 * \text{volume solution}) \quad (1.4)$$

The technical data of four samples is given in Table 1.

Table 1. Technical data of samples.

Sample name	Weight	Solvent	Solvent weight	Calculated solution concentration (Ci)
ASi0001	9 mg	isopropanol	20 ml	450 mg/L
ASi0002	10,5 mg	isopropanol	20 ml	525 mg/L
	10,5 mg	isopropanol	30 ml	350 mg/L
ASi0003	10,6 mg	isopropanol	20 ml	530 mg/L
	16 mg	isopropanol	20 ml	400 mg/L
ASi0004.BA	5.4 mg	isopropanol	20 ml	270 mg/L
	10.5 mg	isopropanol	20 ml	525 mg/L
Cuvettes used for spectrophotometer reading were 10 mm.				

4. RESULTS AND DISCUSSION

The data obtained from the spectrophotometer was collected, plotted using Origin, and then thoroughly analysed. The UV plots representing a significant difference in the absorption patterns of all the samples is showed in Figure 13.

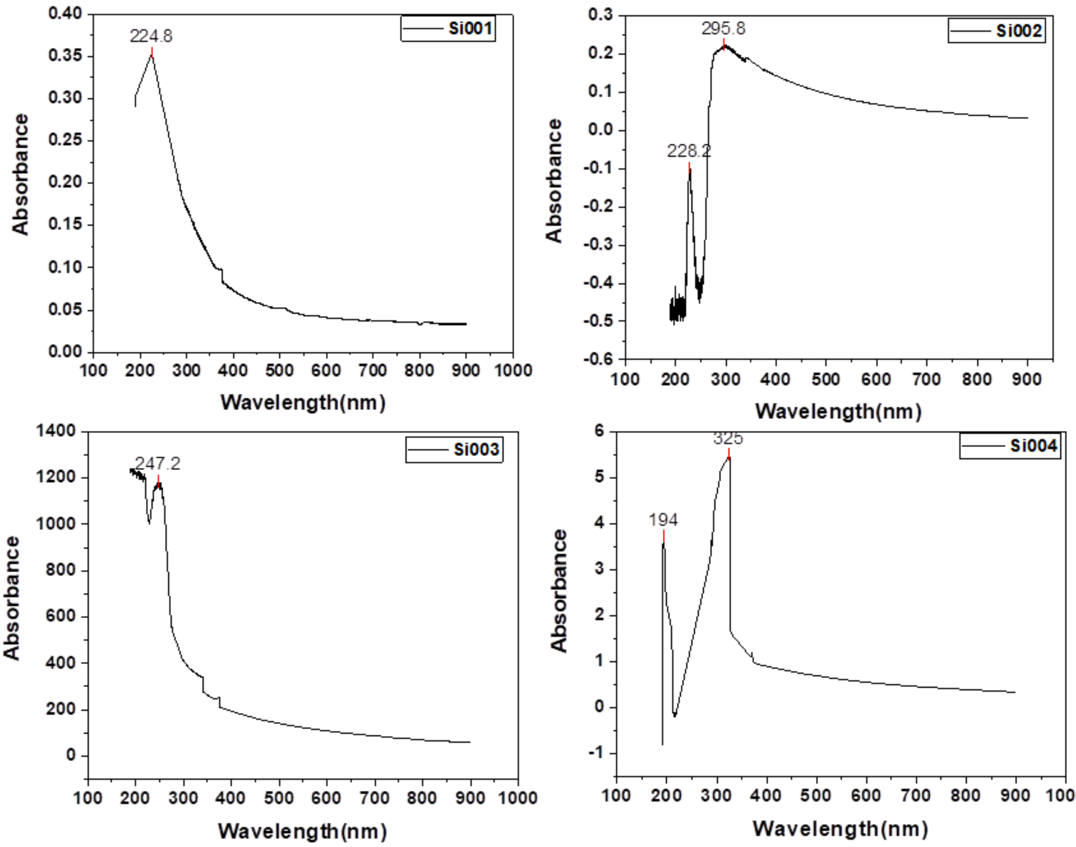


Figure 13. The absorption spectrum of four sol-gel synthesized silicon dioxide samples.

The y-axis represents absorption and x-axis wavelength (nm) of the light in nanometre. The absorption peak is different for every sample. The absorption peaks and calculated data of the samples are shown in Table 2.

Table 2. Absorption peaks and calculation results of the samples.

Sample name	ASi0001	ASi0002	ASi0003	ASi0004.BA
Calculated solution concentration (Ci)	450 mg/L	350 mg/L	400 mg/L	525 mg/L
Calculated molarity	0,0075 M	0,0058 M	0,013 M	0,0087 M
Absorbance	0,35	0,21	1175 ppm = 0,001175	5,4 ppm = $5{,}4*10^{-6}$
Absorption peak	at 224,8 nm	at 295,8 nm	at 247,2 nm	at 325 nm
Molar absorptivity ($M^{-1}cm^{-1}$)	9,346	7,21	0,01765	0,00012
Transmittance	0,45	0,6166	0,9973	0,99
Energy of the photon	5.53 eV	4.2 eV	5.03 eV	3.82 eV
Cuvettes for spectrophotometer reading were 10 mm.				

SiO_2 as a material has a particularity to have low absorption because it has a refractive index of about 1.46 [18,19]. The refractive index describes how fast light travels through the material. A higher refractive index means slower light speed through the material and increases the change of direction of the light inside the material. In SiO_2 light travels 1.46 times slower than in a vacuum. SiO_2 acts as an absorption barrier and its typical application is antireflection coating in combination with other oxides, such as Al_2O_3 [18,20]. The sample ASi001 had the most absorption 0,35 occurring in the UV-C region at 224,8 nm with a photon energy of 5.52 eV. The absorption curve had a rapid decrease after the UV-C region thus reflecting the rest of the light. The sample ASi002 had some initial noise (many data points) and negative absorbance. This means the blank reference (isopropanol) was absorbing more light than the sample. The most absorption 0,21 was occurring in the UV-B region at 295,8 nm with the photon energy of 4,2 eV. The absorption curve decreased slightly after the UV-B region. Very low absorption occurred in the visible light spectrum (400-

700nm) and infrared light spectrum (>700nm). The sample ASi003 had very low absorption 0,001175 occurring in the UV-C region at 247,2 nm with a photon energy of 5.03 eV. The absorption curve decreased rapidly after the UV-C region. Very low absorption is due to the SiO_2 insulator characteristics. SiO_2 has a high bandgap energy approx. 7.52 to 9.6 eV [21]. The photon with the energy of 5.03 eV cannot excite enough the valence band electrons to jump into the conduction band. The sample ASi004BA had the least absorption $5,4*10^{-6}$ occurring in the UV-A region at 325 nm with the lowest photon energy of 3.82 eV. This sample had artefacts in the graph. So it can be stated that this sample is not pure and this contributed to the formation of artefacts. The absorption curve decreased rapidly after the UV-A region but remained almost constant in the visible and infrared light spectrum at a very low level. The samples ASi0002 and ASi0003 are the most promising from these results, as they showed round peak absorption breakup curves. Low absorbance mainly occurred in the energetic UV regions. No absorption occurred in the visible light spectrum (400-700nm). It can be said that all these samples have no absorption in the visible light spectrum and were reflecting light under the visible light spectrum. This confirms that SiO_2 is a poor absorber and acts more like an absorption barrier and insulator, due to its high bandgap energy.

CONCLUSIONS

This study represents the absorbance studies on different sol-gel synthesized SiO_2 samples. Molar absorptivity compensated that absorbance was measured under standard conditions (cuvettes 10mm and solution molar concentration). Calculated molar absorptivity ($M^{-1}cm^{-1}$) was highest 9,346 for the sample ASi0001, 7,21 sample ASi0002, 0,01765 sample ASi0003 and lowest 0,00012 for the sample ASi004BA. The sample Si0004BA is a very bad absorber and produced artefacts in the absorption spectrum graph, thus indicating this sample might have some impurities. Instead samples ASi0002 and ASi0003 showed absorption in respectively in UV-B and UV-C wavelengths with absorbing photon energy 4,2 and 5,03 eV at 295,8 and 247,2 nm-s. Bandgap energies of the samples were calculated by applying Planck´s constant. The sample ASi0001 had the highest bandgap energy 5.51 eV. Even energetic UV photon energy cannot excite enough the SiO_2 electrons in the valence band to jump into the conduction band. High bandgap energy indicates that SiO_2 is a good insulator and does not absorb in the visible spectrum, but reflects. The spectrum graphs for ASi0002 and ASi0003 were the most adequate because the absorption peak curves were round. It would be suggested to analyse them furthermore and to use them for producing a thin film for applying optical measurements. All samples showed bluish purplish UV-light absorption and no absorption under the visible light spectrum. This study indicates the efficiency of SiO_2 nanomaterials as an active back layer in solar cells.

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ÜLDKOKKUVÕTE

RÄNIDIOKSIIDI NANOOSAKESED JA NENDE RAKENDUS PÄIKESEPANEELIDES

Ränidioksiid (SiO_2) on keemiliste elementide räni (Si) ja hapniku (O_2) kombinatsioon. See on Maal väga laialt levinud materjal peamiselt kvartsi ja liiva kujul. Ränidioksiidi kasutatakse dopeeritud pooljuhtelement räniplaatide katmiseks päikesepaneelide fotogalvaanilistel elementidel. See aitab pinda passiveerida, st väldib pooljuhtelemendi räni oksüdeerumist ning ühtlasi kaitseb seda väliskeskkonna mõjude eest. Samuti kasutatakse ränidioksiidi valguse peegeldumise vähendamiseks või siis soovitud peegeldumise saavutamiseks kombinatsioonis ainetega, millel on erinev refraktsiooniindeks. Puhta amorfse pooljuhtelemendi ränipinna passiveerimine võimaldab säilitada, tõsta fotogalvaanilise elemendi kasutegurit ning vähendada võimalikke kadusid. Fotogalvaanilises elemendis on levinuim elektrienergia tekkimine valguskvantide ehk footonite toimel. Sellist elektrienergia tekkimist nimetatakse ka ventiilfotoefektiks, mis toimub p- ja n-tüüpi dopeeritud pooljuhi (räni) p-n siirdele langevate footonite toimel. Fotogalvaanilised elemendid jaotuvad tootmisviisi järgi generatsioonideks: esimene, teine ja kolmas generatsioon. Esimene generatsioon baseerub kristallilisel ränil, teine generatsioon põhineb amorfsel ränil ning kolmas generatsioon kiletehnoloogial (pooljuhtelement räni kaetakse üliõhukese materjalikihiga nt. ränidioksiid). Tsooniteooria kohaselt on ränidioksiidi keelutsoon lai. SiO_2 keelutsooni energia (valentsitsooni ja juhtivustsooni vahe) on vahemikus 7,52 kuni 9,6 eV (elektronvolt), mis sõltub Si-O-Si sidemenurgast ja pikkustest.

Käesoleva töö eesmärk oli analüüsida UV/Vis spektrofotomeetri abil nelja erinevat sool-geel meetodiga Eesti Maaülikooli Tehnikainstituudi laboris sünteesitud SiO_2 proovi. Kui mingile ainele lasta peale valgus, siis valgus saab kas neelduda, ainet läbida, peegelduda või hajuda. Seega proovide analüüsimine UV/Vis spektrofotomeetri abil oli parim meetod ning võimaldab leida, milliseid lainepikkusi antud nanomaterjal neelab. Neeldumise mõõtmisteks UV/Vis spektrofotomeetris kasutati referentslahustit isopropanooli ning seejärel SiO_2

proovide lahuseid. Kõikide SiO_2 proovide lahuste valmistamiseks kasutati lahustina isopropanooli ning arvutati lahuste kontsentratsioonid. SiO_2 optilisi omadusi uuriti neeldumisspektri kaudu ja andmeid töödeldi tarkvaras nimega „Origin“, et joonistada iga proovi jaoks neeldumisspektri graafikud. Iga SiO_2 proovi jaoks tehti lihtsustatud arvutused, kasutades Beer-Lamberti seadust. Valguse neeldumine ja läbilaskvus varieerus erinevate SiO_2 proovide nanoosakeste kontsentratsiooniga lahuses ja kasutatud küvettidest. Molaarne neeldumistegur kompenseeris, et valguse neelduvus mõõdeti standardsetes tingimustes (küvetid 10 mm st optiline teepikkus ja lahuse molaarne kontsentratsioon). Arvutatud molaarne neeldumistegur ($M^{-1}cm^{-1}$) oli proovil ASi0001 suurim 9,346, proovil ASi0002 7,21, proovil ASi0003 0,01765 ja madalaim proovil ASi004BA 0,00012. Proov Si0004BA on väga halb absorbeerija ja tekitas neeldumisspektri graafikus artefakte, mis näitab, et sellel proovil võib esineda lisandeid. Selle asemel esines proovidel ASi0002 ja ASi0003 neeldumist vastavalt UV-B ja UV-C lainepikkustel absorbeerides footoni energiat 4,2 ja 5,03 eV (elektronvolt) lainepikkustel 295,8 ja 247,2 nm (nanomeeter). Kõikide SiO_2 proovide footonite neeldumisenergiad arvutati Plancki konstandi abil. Proovil ASi0001 oli kõrgeim footoni neeldumisenergia 5,51 eV (elektronvolt). Isegi ultraviolettkiirgusel footoni energia neeldumine ei suuda SiO_2 valentsitsooni elektrone piisavalt ergastada, et need ületaksid keelutsooni ning toimuks nende üleminek juhtivustsooni. Kõrge keelutsooni energia ränidioksiidil näitab, et see on hea dielektrik ja see ei neela valgust nähtavas spektris (400-700 nm), vaid peegeldab. ASi0002 ja ASi0003 spektrigraafikud olid kõige asjakohasemad, kuna nende neeldumisgraafikute kõverate tipud olid kumerad ning sujuvad. Töö tulemusena soovitaksin neid proove veel edasi analüüsida ja kasutada neid õhukese kile tootmiseks, selleks, et mõõta nende optilisi parameetreid. Kõik analüüsitud SiO_2 proovid näitasid sinakaslillat UV-valguse neeldumist ja nähtava valguse mitteneeldumist. See töö näitab ja kirjeldab SiO_2 kui nanomaterjali, mida saaks kasutada päikeseelementides.

APPENDIXES

LIHTLITSENTS

Lisa 1. Lihtlitsents lõputöö salvestamiseks ja üldsusele kättesaadavaks tegemiseks ning juhendajate kinnitus lõputöö kaitsmisele lubamise kohta

Mina, Indrek Alberg, sünniaeg 20.04.1991,

1. annan Eesti Maaülikoolile tasuta loa (lihtlitsentsi) enda koostatud lõputööle

   Absorption Spectroscopy Studies of Silicon Dioxide Nanoparticles and Their Applications in Solar Cells,

   mille juhendajad on Prof. Protima Rauwel, Prof. Erwan Yann Rauwel ja Rohit Kumar,

   1.1. salvestamiseks säilitamise eesmärgil,
   1.2. digiarhiivi DSpace lisamiseks ja
   1.3. veebikeskkonnas üldsusele kättesaadavaks tegemiseks kuni autoriõiguse kehtivuse tähtaja lõppemiseni;

2. olen teadlik, et punktis 1 nimetatud õigused jäävad alles ka autorile;

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Lõputöö autor Indrek Alberg (allkirjastatud digitaalselt)

Tartu, 28/05/2021

Juhendajate kinnitus lõputöö kaitsmisele lubamise kohta

Luban lõputöö kaitsmisele.

Prof. Protima Rauwel (allkirjastatud digitaalselt) 28/05/2021

Prof. Erwan Yann Rauwel (allkirjastatud digitaalselt) 28/05/2021

Rohit Kumar (allkirjastatud digitaalselt) 28/05/2021