Absorption Depth Profile of Silicon Substrate in the Presence of Copper Nanoparticles: A Study on Simulation and Fabrication Thereof

Mohammad Kamal Hossain[1]

[1]Interdisciplinary Research Center for Renewable Energy and Power Systems (IRC-REPS), Research Institute, King Fahd University of Petroleum & Minerals (KFUPM), Dhahran 31261, (Kingdom of Saudi Arabia)

Abstract

Copper nanoparticles have attracted interest in the field of solar cells due to their potential for improving light absorption, plasmonic effects, cost-effectiveness, non-toxicity, and simplicity of production and integration. In this context, simulative prediction of such system facilitates efficient device fabrication. In this work, finite-difference time-domain (FDTD) analysis was carried out to understand the influence of copper nanoparticles within silicon (Si) substrate. An FDTD model, "Copper nanoparticles array as 3×3 on c-Si slab" was developed and absorption depth profiles were extracted at several incident wavelengths of solar spectrum for different interparticle gaps of copper nanoparticle array. It was noted that absorption distribution within Si substrate depended on incident wavelengths of solar spectrum as well as distribution of copper nanoparticles. To realize the results obtained in FDTD simulation, a simple strategy was devised to fabricate copper nanoparticulate using sputtering technique. High resolution field emission scanning electron microscopic (FESEM) images revealed that as-fabricated copper nanoparticles were in the range of 80-100 nm in diameter. FESEM-aided energy dispersion spectroscopy confirmed the elemental composition of the copper nanoparticulate.

Keywords: Copper nanoparticles, FDTD simulation, absorption depth profile, sputtering deposition

1. Introduction

Most of the photovoltaic panels are silicon (Si)-based, although conventional Si-based solar cells are neither cost-effective or efficient enough. However, thin film solar cells, particularly third generation solar cell, have enormous cost-cutting and efficiency-boosting potential (Lee and Ebong, 2017; Abdullah et al., 2019). In this context, down-shifting materials are very promising to convert higher-energy photons such as ultraviolet (UV) photon into lower-energy photons (McKenna and Evans, 2017). The process not only supports the increased photocarriers generation, but also deals with UV protection of the photoactive devices (Gheno et al., 2018). Copper is one of the most commonly utilized materials, as it is simple to acquire both chemically and through physical deposition techniques (Cemin et al., 2016). Copper nanoparticles can improve the light absorption capability of solar cells (Shreya and Varshney, 2021; Jhuang et al., 2021). They can be added to the active layer of a solar cell, such as the bulk heterojunction (BHJ) or the perovskite layer, to boost solar absorption. Copper nanoparticles have plasmonic characteristics that lead to interaction with light at certain wavelengths. This interaction has the potential to increase light trapping and absorption within the solar cell, resulting in higher efficiency (Chen et al., 2021). Copper is a plentiful and relatively inexpensive substance when compared to noble metals such as gold or silver. As a result, copper nanoparticles are an appealing option for improving solar cell performance without considerably raising production costs (Shaikh et al., 2021). Copper is non-toxic, which is advantageous for ecologically friendly solar cell technology. It eliminates worries about the use of harmful compounds in the manufacture of solar cells. Chemical reduction, solvothermal approaches, and solution-based processes can all be used to create copper nanoparticles (Parveen et al., 2016). They can be included into the structure of a solar cell via ink formulations, nanoparticle dispersions, or thin film deposition processes.

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In this study, a finite difference time domain model "Copper nanoparticles arrayed as 3×3 on c-Si slab" was used to understand the photon absorption within the Si layer. Although several incident solar spectrum wavelengths were employed throughout the simulations, three specific wavelengths were in focus: one in the near UV (400 nm), one in the visible range (800 nm), and another in the near IR (i.e. 1100 nm). A simple strategy was devised to fabricate copper nanoparticles using sputtering technique followed by further treatment. Topographic and elemental confirmation were carried out using high resolution field emission scanning electron microscope (FESEM) and FESEM-aided energy dispersion spectroscopy (EDS) respectively**.**

2. Method and experimental

A typical thin film solar cell illustrating possible inclusion of functional nanoparticulate has been shown in Fig. 1a. To realize the concept, it was inevitable to fabricate Cu nanoparticulate as an initial layer. A one step process has been devised in this work as mentioned in Fig. 1b. Fig. 1b represents a freehand schematic demonstrating steps involved in fabricating copper nanoparticulate. Copper target of 2 inch in diameter (99.99% purity) were purchased from ACI alloy, Inc. and used as received without any further treatment. The chamber base pressure and working pressures were kept about 1.7×10-5 torr and 2.8×10-3 torr, respectively in Ar flow rate of 30 SCCM. The deposition power was maintained at 30 W and an in-built thickness monitor was set to 50 nm. Afterward, the deposited films were annealed in a tube furnace (model MTI Corporation OTF-1200X) at 600 °C for 2 hrs with a heating rate of 20 °C/min. This is to be understood that here in this work, an attempt has been taken to fabricate copper nanoparticulate that can be further utilized as initial layer in thin film solar cell design. An FDTD simulation tool (Lumerical Solution, ver 8.6) was utilized to extract absorption depth profiles at different wavelengths of solar spectrum for different interparticle gaps as shown in Fig. 1c. The choice of nanoparticle size in FDTD simulation, i.e. 100 nm in diameter was based on FESEM confirmation. Although several incident wavelengths of solar spectrum were used for interparticle gaps of 0, 1 and 3 nm, three specific wavelengths of solar spectrum 400, 800 and 1100 nm were chosen as demonstrated in the later part of the text.

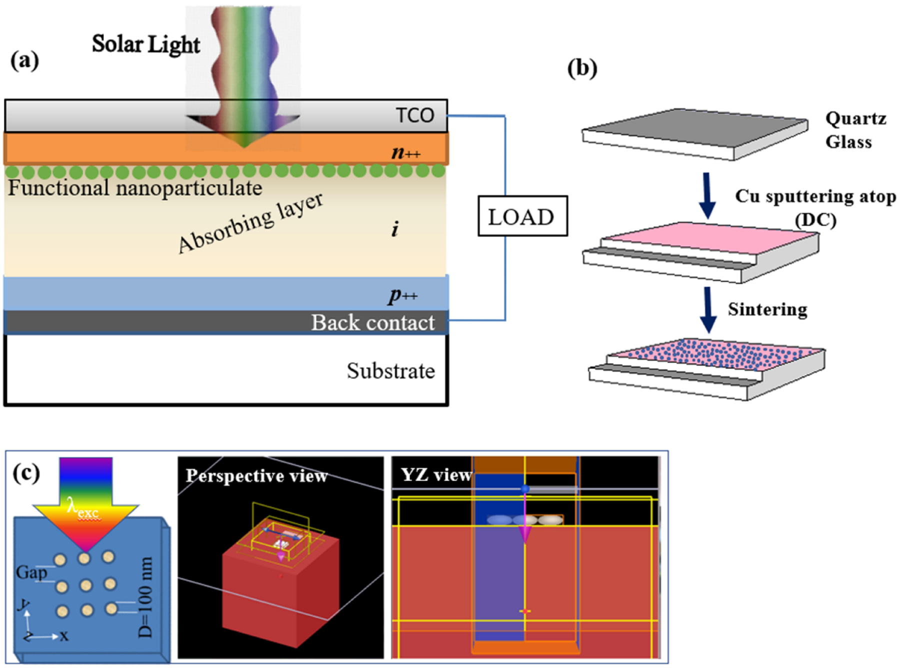

Fig. 1: (a) A tyypical thin film solar cell illustrating possible inclusion of functional nanoparticulate, (b) Free-hand schematic showing the mechanism adopted in this investigation to achieve Cu nanoparticulate to be included within thin film solar cell design and (c) FDTD model used in simulation; left-pane: free-hand schematic, middle-pane: perspective view and right-pane: YZ view showing the position of monitors.

3. Results and discussion

Understanding and adjusting solar cell absorption depth profiles is critical for reaching high conversion efficiencies. Continuous efforts are made to investigate innovative materials, device designs, and light trapping technologies in order to increase light absorption and overall performance of solar cells. The depth at which light is absorbed inside the active layer of a solar cell is referred to as the absorption depth profile. It is a critical factor that influences the overall efficiency and performance of the solar cell. Figure 2a–c show absorption depth profiles of interacting copper nanoparticles array at incident solar wavelengths of 400, 800 and 1100 nm respectively along with maximum and average power. It is noteworthy that at lower incident wavelength of solar spectrum (e.g. 400 nm), underneath Si was found more affected whereas at longer wavelengths such as 800 and 1100 nm lower absorption depth profiles were observed. In this context, zoon-in views of the absorption depth profile within Si were extracted and were shown in corresponding insets. In the case of shorter wavelength such as at 400 nm of solar wavelength, more than half of the active layer that is just below the Cu nanoparticulate was found to be enhanced. However for longer wavelengths such as at 800 and 1100 nm of solar wavelength most of the underneath Si was moderately enhanced. Absorption depth profiles for interparticle gaps of 1 and 3 nm have been extracted at 400, 800 and 1100 nm of incident wavelengths. To the extend, maximum absorption power and average power have been recorded for interparticle gaps of 0, 1 and 3 nm at 400, 800 and 1100 nm of incident wavelengths of solar spectrum.

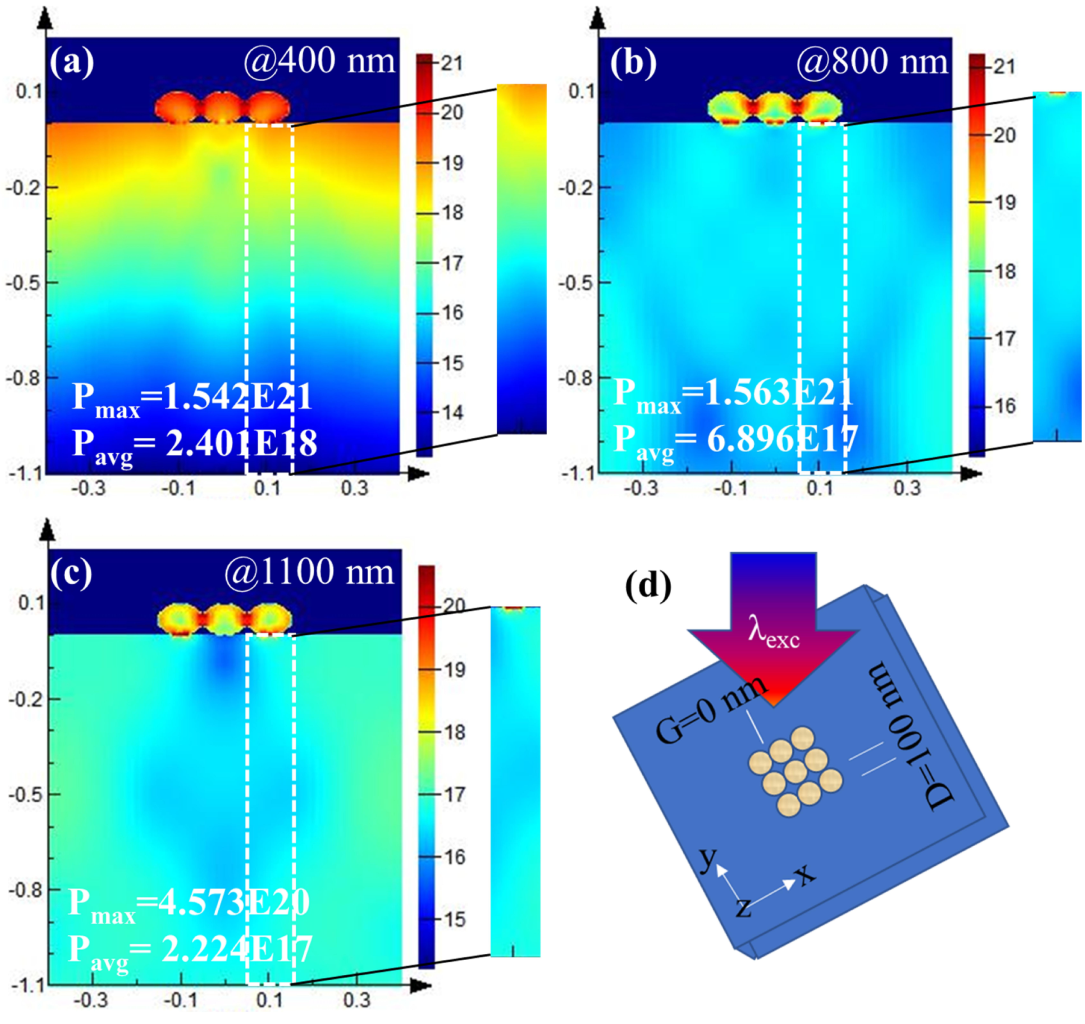

Fig. 2: (a)-(c) Absorption depth profile of interacting copper nanoparticles array at 400, 800 and 1100 nm respectively and (d) free-hand schematic to represent model geometry (not to the scale) used in FDTD simulation. Corresponding color bar represents the absorption intensity in log scale.

Apart from improved absorption and energy quenching, the nanoparticulate interparticle gap has a significant effect on plasmon coupling driven properties. When nanoparticles are close together, the plasmon resonances of surrounding particles may be tuned to meet specific demands. The specific impact is determined on the nanoparticles' size and shape, as well as the interparticle spacing. A decreased interparticle gap results in increased light absorption at shallower depths as shown in Fig. 2a-c.

Figure 3a–c show absorption depth profiles of copper nanoparticles array of 1 nm interparticle gap along with maximum and average power at incident solar wavelengths of 400, 800 and 1100 nm respectively. One can notice that at lower incident wavelength of solar spectrum, underneath Si was found more affected whereas at longer wavelengths such as 800 and 1100 nm lower absorption depth profiles were observed. Similar to interacting Cu nanoparticle array, at shorter wavelength, more than half of the active layer was found to be influenced as displayed in Fig. 3a. However, the majority of the underneath Si was only slightly improved for longer wavelengths, such as at solar wavelengths of 800 and 1100 nm as shown in Fig. 3c and Fig. 3d. In this regards, zoon-in views of the absorption depth profile within Si were extracted and were shown in corresponding insets.

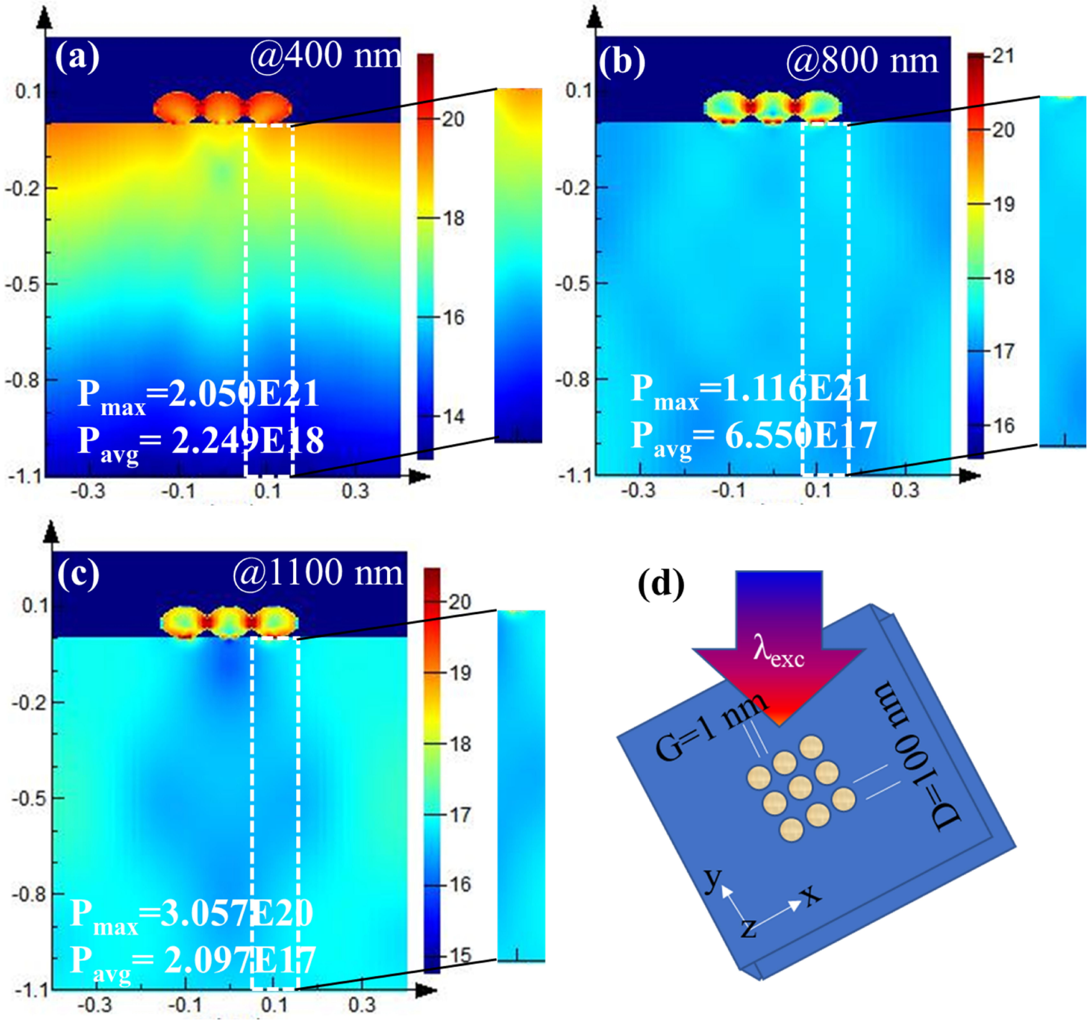

Fig. 3: (a)-(c) Absorption depth profile of copper nanoparticles array of 1 nm interparticle gap at 400, 800 and 1100 nm respectively and (d) free-hand schematic to represent model geometry (not to the scale) used in FDTD simulation. Corresponding color bar represents the absorption intensity in log scale.

In the case of higher interparticle gaps, the absorption depth profile distributions started to change within Si active substrate place to place. Figure 4a–c show absorption depth profiles of copper nanoparticles array of 3 nm interparticle gap along with maximum and average power at incident solar wavelengths of 400, 800 and 1100 nm respectively. At shorter wavelength of solar spectrum, underneath Si was found more or less similar to those obtained at interacting and closely packed Cu nanoparticles array. However, at longer wavelengths such as 800 and 1100 nm lower absorption depth profiles were observed to be spread throughout the underneath layer. Zoon-in views of the absorption depth profile within Si as shown in corresponding insets represent the scenario. The effect of interparticle gap on the absorption depth profile of nanoparticles is a complex phenomenon that depends on the size, shape, and arrangement of the nanoparticles. The interparticle gap can influence the plasmon resonances, leading to changes in the absorption spectrum and depth profile.

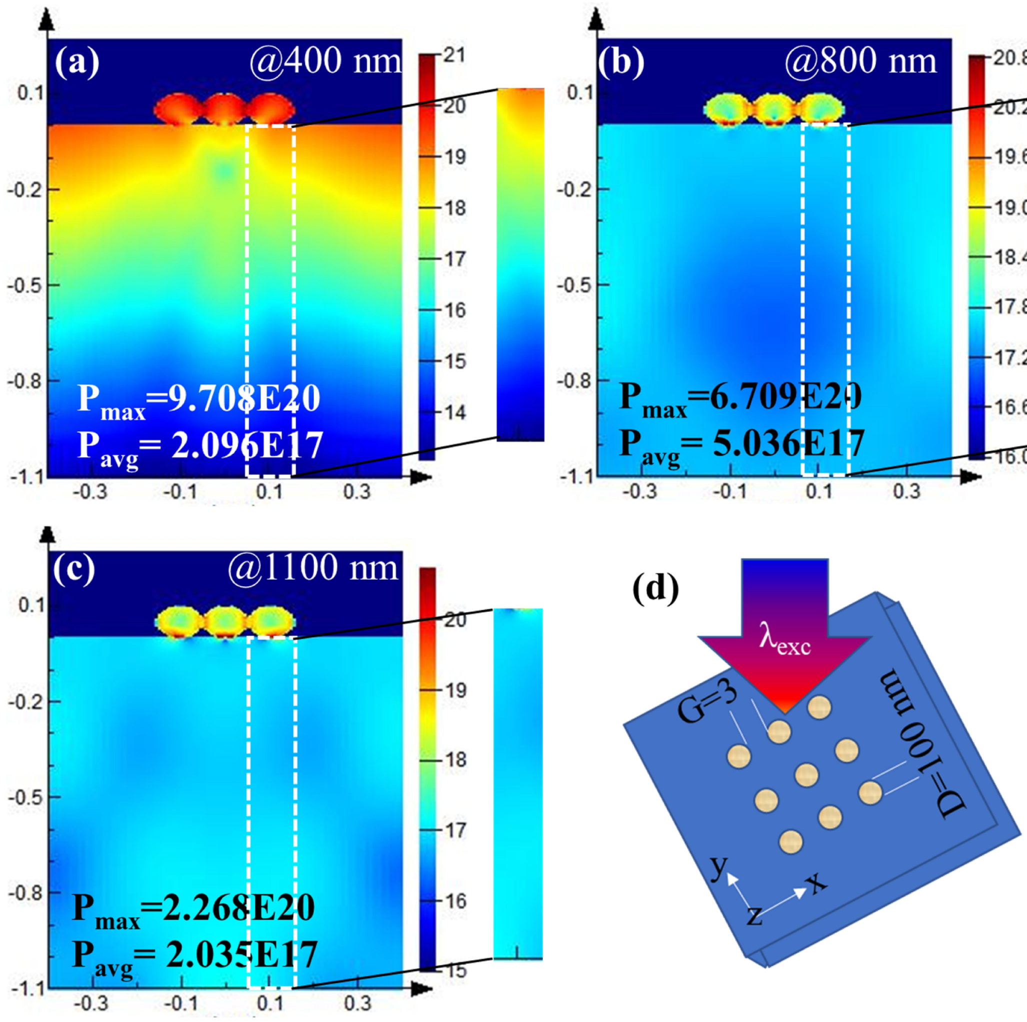

Fig. 4: (a)-(c) Absorption depth profile of copper nanoparticles array of 3 nm interparticle gap at 400, 800 and 1100 nm respectively and (d) free-hand schematic to represent model geometry (not to the scale) used in FDTD simulation. Corresponding color bar represents the absorption intensity in log scale.

An attempt was taken to fabricate copper nanoparticles as shown in Fig. 5a. Such multifunctional layer can be integrated in substrate and superstrate type thin film solar cell as explained in previous study (Hossain and Mukhaimer, 2020). A high resolution FESEM micrograph of copper nanoparticulate was shown in Fig. 5b. Inset (i) of Fig. 2b reconfirmed an average diameter of copper nanoparticles of ca. 80 nm. SEM-aided EDS was carried out to confirm elemental composition of the film as shown in inset (ii) of Fig. 5b.

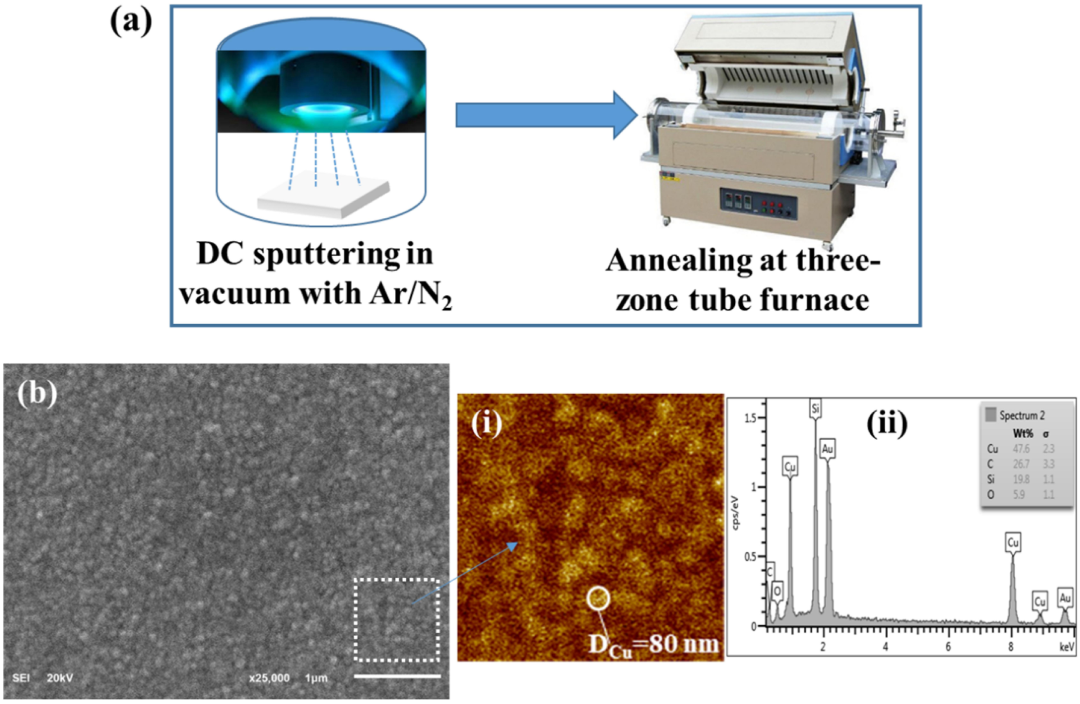

Fig. 5: (a) Free-hand schematic of thin film growth using sputtering technique and subsequent treatment and (b) FESEM micrograph of copper cluster fabricated on glass; inset (i): Zoom-in view of a selected area (1 µm × 1 µm) as marked by the white dashed square in Fig. 2b and inset (ii): SEM-aided EDS measurement of the same nanoparticulate.

4. Conclusion

FDTD simulation for a model "Copper arrays on c-Si slab" showed that absorption profile of the underneath Si subtracted get affected and depend highly on the incident wavelengths of solar spectrum as well as interparticle gaps of copper array. At lower incident wavelength of solar spectrum (e.g. 400 nm), absorption distributions were more intense in Si whereas at longer wavelengths such as 800 and 1100 nm lower absorption depth profiles were observed. When particles are near together, they interact and generate scattering and interference effects. These influences modify the path of light and hence the absorption depth profile distribution. The fact was further demonstrated by varying the interparticle gaps from 0, 1 to 3 nm of the model geometry "Copper arrays on c-Si slab". To realize the potential of such copper nanoparticles in thin film solar cell, an attempt was taken to fabricate copper nanoparticulate in such a way so that the layer can be utilize further to be considered as an initial layer in thin film solar cell design. FESEM image confirmed the diameter of as-fabricated copper nanoparticles in the range of 80-100 nm.

5. Acknowledgement

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