Analysis of Incorporation of Ion-Bombarded Nickel Ions with Silicon Nanocrystals for Microphotonic Devices

L. Natrayan, P. V. Arul Kumar, S. Kaliappan, S. Sekar, Pravin P. Patil, R. Jayashri, and E. S. Esakki Raj

1Department of Mechanical Engineering, Saveetha School of Engineering, SIMATS, Chennai, 602105 Tamil Nadu, India
2Department of Mechanical Engineering, Bharath Niketan Engineering College, Aundipatti, 625531 Theni, Tamil Nadu, India
3Department of Mechanical Engineering, Velammal Institute of Technology, Chennai, 601204 Tamil Nadu, India
4Department of Mechanical Engineering, Rajalakshmi Engineering College, Rajalakshmi Nagar Thandalam, Chennai, 602105 Tamil Nadu, India
5Department of Mechanical Engineering, Graphic Era Deemed to Be University, Bell Road, Clement Town, 248002 Dehradun, Uttarakhand, India
6Department of Electronics and Communication Engineering, Rajiv Gandhi College of Engineering and Technology, Kirumampakkam, Puducherry 60740, India
7Department of Mechanical Engineering, Dambi Dollo University, Ethiopia

Correspondence should be addressed to L. Natrayan; natrayan07@gmail.com, S. Kaliappan; mahesh2675@gmail.com, and E. S. Esakki Raj; essakkiraj@dadu.edu.et

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Nanotechnology is playing a greater role in biomedical engineering. Microphotonic technology is on another side, having faster growth with more requirements. The nanocrystals are a part of nanotechnology which uses silicon for manufacturing. These silicon nanocrystals have the optical property mostly used in microphotonic devices. Silicon nanocrystals are of biocompatibility with less toxicity. Therefore, the advancement in the silicon nanocrystal helps develop more microphotonic devices for biological purposes. One critical factor of silicon nanocrystal is the surface defects or surface imperfections. Surface passivation is the method employed for rectifying this disadvantage of silicon nanocrystal. Another major thing is that silicon nanocrystals are size dependent. So proper variation on the surface is required for yielding high performance of the nanocrystal. After characterizing the surface of the silicon nanocrystal, ion bombardment can occur. Nickel is a lustrous white chemical element which is less reactive when it is of a smaller size. So ion bombardment of nickel ion on the surface of the silicon nanocrystal can be done to improvise the performance of the microphotonic devices. Nearly there is an excess of 20 a.u. of photoluminescence intensity yielded. The relative fluorescence is also increased by 150 a.u. This research work enhanced the silicon nanocrystal using ion bombardment of nickel ion, which increased energy traps resulting in more intensities.

1. Introduction

Microphotonic technology helps transmit, detect, and process light from one millimeter to ten-millionth of millimeter scale devices [1]. Its applications include lasers, biomedical, aircraft, and sensors. This technology uses the great properties of nanocrystals at atomistic levels, mainly used in biomedical applications like drug delivery and internal organ study [2]. The siltation ion has an optical emission property which helps make nanocrystals. The silicon nanocrystals can be manufactured in two ways, top- and bottom-up approaches [3]. The defects on the surface lead to a reduction in the recombination of electron-hole pairs [4]. Many approaches were carried out for surface passivation of silicon nanocrystals [5]. Meier and Lorke investigated silicon nanocrystal’s dark and bright excitation modes and introduced a device based on electroluminescence [6]. Sigmund studied the collision of cluster atoms and its sputtering effects in...
1989 [7]. Vasyl et al. analyzed silicon in the midinfrared region and surface optical phonon mode of SiO$_2$ [8]. The electronic sputter and intensities obtained during the bombardment of nickel ions showed sharp spectral intensities in different wavelengths were analyzed by Jadoual et al. [9]. From the survey, it is clear that some of the defects in the surface of the silicon nanocrystals lead to deviations in the radiations and reduced intensities [10]. In this paper, the ion bombardment of nickel ions is incorporated into the surface of the silicon nanocrystals to increase the intensity range.

In such studies, various kinds of substrate materials such as monoelemental, binary, and multicomponent materials have been utilized. Out of the monoelemental materials, Si and Ge substrates were used extensively [11]. The choice of such material, especially Si, is its easy availability, low cost, and applicability in a broad range from a technological aspect. Moreover, among the semiconducting materials, Si has been regarded as a paradigmatic entity for designing experimental and theoretical models. Different groups have furnished a variety of patterns on Si surface including ripples, dots, and holes, which can be easily reproducible [12]. Upon bombardment, it creates numerous lattice defects on the sample’s near surface region, thereby destroying the crystal structure [13]. For the ion beam-induced patterning experiments, the selection of ion type employed also plays a crucial role. The interaction of the energetic ion with the solid surface results in the transfer of energy and momentum from the ion to the lattice atoms present inside the solid material, leading to a series of primary and secondary collisions within the material [14]. After losing all its energy, the ion ultimately comes to rest and gets implanted. The collisions termed collision cascade encourage the formation of interstitials and vacancies within the solid, generating a stochastic disorganized and unstable region at the near-surface depth [15].

During ion bombardment, some lattice atoms undergoing collision may knock out from the material, causing surface erosion, provided their kinetic energy exceeds the surface binding energy [16]. As the solid is subjected to continuous ion irradiation, after the bombardment time exceeds a certain threshold, a highly disordered state rich in lattice defects is developed, leading to surface amorphization [17]. With high production scalability from extremely small regions to large areas, the sputtering phenomenon is the foundation of numerous surface coating processes in industrial and commercial activities [18]. Also, the IBS technique is used in various surface analytical measurements as a prerequisite tool. For instance, in the case of transmission electron microscopy (TEM) measurements, the required sample thickness should be thin enough for the electrons to transmit through it [19]. With the sputtering method’s help, gradual surface erosion occurs, leading to surface thinning, and the sample with a precise thickness is finally achieved [20].

Ion bombardment is the new technique where the ions are embedded on the surface of the silicon nanocrystal. Novel of this research work enhanced the silicon nanocrystal using ion bombardment of nickel ion which increased more energy traps resulting in more intensities. Many methods like doping, adsorption, and CVD are carried out.

2. Materials and Method

2.1. Silicon Nanocrystals. The nanoparticles are as different forms like nanowires, nanocomposites, and nanopowder. The nanocrystals are particles with either a single or poly-crystalline structure. Silicon is an abundant element available on the earth [21]. The silicon can be made as nanocrystals using different approaches [22]. The size of the nanocrystals varies from 2 to 20 nm. The density can be measured as 1012 cm$^2$ ± 2. It is manufactured in two ways: the top-down and the bottom-up approaches. In the top-down approach, three types are electrochemical etching, laser ablation and mechanical milling. It is a simple and easy method of manufacturing nanocrystals [23]. Small particles are used in the bottom-down approach to make the silicon nanocrystals [24]. It involves the combustion template, microwave, and hydrothermal methods for manufacturing. It is mainly used way to produce fluorescent silicon nanocrystals [25]. The surface state of the silicon nanocrystals needs to be passivated to improve the radiation property [26]. The surface of the silicon nanocrystals has many imperfections and defects which need to be rectified. Many methods were involved. The surface defects are filled using different particles and tried to increase the recombination rates of the silicon nanocrystals [27]. The silicon nanocrystal with polymer composites was investigated, acting as the interfacial element between the surface state of the nanocrystal and other substrates. The polymer composites reduce the silicon’s reaction rate to the atmosphere [28]. The ultrahigh stability produced by the polymer composite with the silicon nanocrystals prolongs the lifetime of the photonic devices even for a year. With the metal composites, the silicon nanocrystal’s energy gaps become wider thus increasing the fluorescence property [29]. The nonmetal and hydroxide composites are also used along with the nanocrystals, which improve the fluorescence resonance property of the beam [30]. The silicon nanocrystals are luminescent display devices, solar energy cells, biomedical applications, drug delivery, light emitting devices, carrier materials, storage devices, micro- and integrated semiconductors, floating gate memory device QD lasers, and agricultural applications [31]. The main properties of silicon nanocrystals are less toxicity, stabilized quality, stable photoluminescence, good fluorescence, large amount of crystallization, substantial dispersibility, more functional groups, catalytic properties, multicolour emissions, feasible large-scale productions, good biocompatibility, cost-effectiveness, being eco-friendly, cytotoxicity, and cytocompatibility [32]. The optical property of the silicon nanocrystals can be studied with the help of luminescence. The luminescence quality depends on the quantum confinement effects, nanocrystal surface characterization, siloxane formation, and spatial confinements [33].

2.2. Ion Bombardment. The bombarding of ions on any material’s surface to overcome defects is called ion bombardment. It happened in the form of beam, clustering, or sputtering way. It also helps in the removal of impurities from the surfaces. It helps nucleate the surface of metallic ions with substrates [34]. The ions occupy the surface’s defect
area, which involves the production of more electron hole pairs in the recombination process. The cost of ion bombardment is quite high as it requires more kinetic energy to produce the beam of ions [35].

2.3. Optical Properties of Nickel Ions. The nickel ions usually occupy the tetrahedral and octahedral positions in the crystalline structures. It adds more stability to the polycrystalline structure in which it is embedded. Usually, for silicon nanocrystals, octahedral occupancies are more important [36]. The Ni$^{+2}$ ions are of octahedral type. The chemical bond of nickel ions can be calculated using the following formula:

$$h = \frac{1 - \beta}{k_{Ni^{+2}}},$$  \hspace{1cm} (1)

where $k_{Ni^{+2}} = 0.12$ for nickel ions. This is the main application of nickel ions in quantum applications and biomarking.

3. Experimental Procedure

3.1. Ion-Bombarded Nickel Ions. The setup for the ion bombardment of nickel ions is carried out. The beam of 5 keV of nickel ions is directed at the surface of the silicon nanocrystals. The beams contain two microamp intensities with a cross-section of 1 mm$^2$. The sample holder was rotated to sputter the nickel ions evenly on the surface of the silicon nanocrystals. The sputter cycle takes 1 min for a cycle to complete. The light emission was studied using the monochromator [37]. The diameter of the ion beam was lustrous materials which can be mm according to the aperture size. The nickel ions are oxidized easily. Usually, the nickel, as a very small particle, reacts more than the larger particles. Here, the nickel ions are emitted as beams on the surface of the silicon nanocrystals to be more reactive in its imperfect areas. They are formed like a cluster on the defect sites, so they will not be oxidized. The nickel ions are ferromagnetic at room temperature [38]. So, the arrangement of nickel ions in the different states of the crystalline can also be carried out.

3.2. Mechanism. The optical property of silicon nanocrystal usually occurs during the energy states’ transition. The quenching of the energies in the different states produces light of different spectra. The quenching usually presents for a particular period [39]. More electron-hole pairs are generated on the excitation mode of the silicon nanocrystals. The electron-hole pairs generated start recombining to form more energy. The formation electron-hole pair needs some energy, and recombination starts to emit energy in the form of photons [40]. The colour of the photons depends on the wavelength of the energy emitted. The photoluminescence of the silicon nanocrystal can be enhanced by increasing the electron-hole pair recombinations. There is a state in the silicon nanocrystal called quasistates that emits energy but is limited to photons. So the main thing to be noted is that the electron should be moved to an excited state from the valence state without losing energy [41]. The energy gap is the main parameter for wavelength measurement.

The energies of the different states are the energy obtained from different orbital energy. As long as ions form on the surface of the silicon nanocrystals, the recombination process will take place at a high amount. So, to increase the silicon nanocrystals’ photoluminescence, more ion formations are very much required [42].

Another thing which needs more attention is the surface defects and imperfections of the silicon nanocrystals. The surface defects and imperfections usually occur during the manufacture of the silicon nanocrystals. The problem caused by the surface defect is that it reduces the performance range of the silicon nanocrystals. The presence of a void reduces the production of electron hole pairs, reducing the recombination rate. So that the photoluminescence quality of the silicon nanocrystals reduces, the empty surface sites need to be analyzed and refilled. The characterization of the surface imperfection and surface defects is more complex. Accurate characterization is difficult to obtain. The maxima and minima on the surface need to be calculated for the process of surface passivation. Once the defects are occupied with the ions, the generation and recombination of electron-hole pairs will increase [43].

This paper proposes a new method of using nickel ions in silicon nanocrystals to improve their photoluminescence. But the main disadvantage of nickel ions is that they are highly reactive when their size is larger. The nickel ions’ size needs to be minimized to have its full advantage. The beam of nickel ions can be used. As the beam, the size of the nickel ions will be very small. When the nickel beam ions of 5 keV intensity are used on the surface of the silicon nanocrystals, it occupies the imperfection and surface defects present in it. After embedding, the nickel ions occupy the octahedral positions of the nanocrystalline silicon structure. The silicon breaks its covalent bond and starts to produce more ions. These ions will start to recombine with nickel ions. But there will be two nickel ions which will react with the silicon having 4 electrons in the valence band. The other two electrons will be left to move freely on the surface of the silicon nanocrystals. These free-moving electrons hit another atom, which starts to lose electrons and forms ions. Therefore, many electrons will be present with fewer holes to recombine. After some durations, the recombination occurs, and more energy will be produced. The darker and brighter excitation modes are studied. The excitons will be settling more time in the excitation states for some duration due to the loss of holes for recombination. After some time, the holes formed to attract the electron. The nickel ion gets settled in the centre of the crystalline structure, increasing the ligand effects.

The presence of more energy traps in the proposed work leads to a more intense output signal. The energy of the photoluminescence will be very high due to the high intensities of the evolution of the photons. Therefore, many wavelengths with high intensity are produced when nickel ions recombine with the silicon crystals for different wavelengths. If the intensity is not up to the desired level, the photoluminescence of that wavelength will be affected. Once the ion bombardment of nickel ions hits the surface of the silicon nanocrystals, it starts to produce immense energy. For
devices like photovoltaic cells, nickel ions act as good adsorbents of light and serve as a good substrate. The silicon nanocrystals are size dependent. The photoluminescence property also depends on the size of the molecule of the silicon and nickel. The size should be average to withstand the ion bombardment processes. Sometimes due to more energy, the ion bombardment of silicon leads to more energy, which destroys other devices in the system. So handling the ion bombardment process should be given more importance. It should be maintained below the avalanche breakdown, which is the cause of the excess energy. The excess energy will increase the device’s temperature due to less resistance. This ion-bombarded nickel ions enter the silicon nanocrystal’s octahedral position, producing good photoluminescence properties for various wavelength regions. Both nickel and silicon elements play a major role in biomedical applications.

4. Results and Discussions

The proposed work is simulated and compared the performance of ion-bombarded nickel in silicon nanocrystal with the normal silicon nanocrystal. The performance is concentrated mainly at 350-400 nm wavelength and analysis. The simulation is carried out considering the size of silicon nanocrystal of 10 nm with a 1 nm height range. The fringe spacing is also considered, which is approximately 0.34 nm. The energy of photons of wavelength is usually $5.7 \times 10^{-19}$ J. The nickel ion bombardment is considered to be randomly distributed on the adsorbent surface of the silicon nanocrystals. The silicon nanocrystals have the surface states considered Poisson distribution for simulation purposes. The simulation is carried out using the values present in Table 1.

Figure 1 shows the number of nickel ions adsorbed on the surface of the silicon nanocrystals. The graph shows that the number of nickel ions absorbed constantly increased during ion bombardment at the initial stage. After 0.6, the absorption rate increases. The absorption rate increases with the increase of time. The direction of the angle of the Bram bombardment needs to constantly vary on the surface of the silicon nanocrystal to maintain uniformity on the surface. In the simulation, poison distribution of nickel ion on the surface site is done. Here, we have taken Ni$^{+2}$ ions; it settles down in the octahedral location of the silicon nano-polycrystalline structure.

Figure 2 shows the plot of wavelength vs. photoluminescence intensity. It is seen that the intensity is increased for the proposed work compared to the normal silicon nanocrystals. Nearly 20 a.u. variation is shown in the plot. This variation in the intensity is mainly due to the introduced nickel ions onto the surface of the silicon nanocrystals. The density of the nickel ion bombarded on the surface makes it less reactive to nature. When the intensity increases, the bandwidth will become narrower. Therefore, the narrower bandwidth with high intensity helps secure communication without loss using photonic devices. The narrower bandwidths can be put together and help transmit wider signals. The energy level on the surface state increases as more ions are ready to recombine. Once the recombination rate increases, the silicon nanocrystals start to emit photon. The energy of the photon should be very high to give more intense signals. The dye-sensitized cells also require highly intensified nanocrystal for functioning.

Figure 3 shows the plot of wavelength vs. the relative fluorescence intensity. The relative fluorescence is the photons released to the amount of energy absorbed. Here, the absorption of nickel ions increases the relative fluorescence

<table>
<thead>
<tr>
<th>Simulation parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nanocrystal diameter</td>
<td>10 nm</td>
</tr>
<tr>
<td>Height</td>
<td>1 nm</td>
</tr>
<tr>
<td>Fringe spacing</td>
<td>0.34 nm</td>
</tr>
<tr>
<td>Energy of photon</td>
<td>$5.7 \times 10^{-19}$ J</td>
</tr>
<tr>
<td>Wavelength</td>
<td>350-400 nm</td>
</tr>
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The intensity of silicon nanocrystals. The silicon nanocrystal radiation decreases with an increase in surface defects and surface imperfections. Due to surface defects, the silicon nanocrystal emits a photon at various unwanted wavelengths. This leads to the loss of energy. The nickel ions bombarded on the surface of the silicon nanocrystal start reacting with the silicon in its crystalline structure. This makes the crystalline structure of the silicon nanocrystal more stable and starts to emit radiations. Nearly 150 a.u. variation is obtained from the proposed work. According to the absorbed energy, only the silicon nanocrystal will emit since the absorption of nickel ion in turn increases the energy on the surface of the silicon nanocrystal by reaction and producing and recombining with the more electron-hole pairs.

The model incorporates ballistic smoothing, curvature-dependent erosion, and ion-enhanced viscous flow as surface phenomena occur during IBS without impurity. But after Fe inclusion, crucial phenomena such as surface tensile stress and preferential sputtering have been integrated in the model. As per the theory, in the presence of Fe, the model predicts that surface stress-induced instability combined with curvature-dependent erosion dominates the ballistic smoothing, resulting in the creation of dot patterns on the surface.

Figure 4 shows the energy vs. intensity plot. The system’s energy increases by increasing the number of electrons so that its capacity to produce more intensity takes place. From the plot, it is clear that energy increased for the proposed work. The energy is needed to emit more photons. Energy is a performance measure of how much a system can produce. The plot shows that the proposed method has more capacity for producing high-intensity photons at a narrow bandwidth.

Furthermore, the tensile stress causes instability that promotes morphological modification, whereas preferential sputtering acts in conjunction with the instability to achieve the compositional modification on the surface.

The energy is required to enhance the device’s photoluminescence and relative fluorescence. The surface defects are bombarded with nickel ions. These nickel ions try to overcome the imperfection and start to react with the silicon on the surfaces. These nickel ions help produce more ionic reactions and give more ions for further reactions. Thus, the energy of the proposed work is enhanced. This results in a structural transition in the overall near-surface region experiencing collision cascade from crystalline to amorphous. Finally, the bombarded atoms in the affected region undergo self-organization to develop various surface structures.

5. Conclusion

The main disadvantage of the silicon nanocrystal is surface defect which is rectified by filling the nickel ions on the surface of the silicon nanocrystal. Thus, the proposed work of nickel ion bombardment on the silicon nanocrystal was analyzed and studied. The transfer of energy between different states was analyzed, which increased the intensity level of the photons released. The relative fluorescence is shown at nearly 150 a.u. which increased compared to the conventional silicon nanocrystal. The photoluminescence intensity was shown at 20 a.u. compared to existing silicon nanocrystal. The energy of 0.2 eV increased for the nickel ion bombarded silicon nanocrystal. The above performance was mainly achieved due to the quenching of the energy states and an increase in the recombination rate of the proposed work. More energy traps were created, which helped increase the silicon nanocrystal’s energy. The confinement of different orbital energy helps the electron jump from one state to another, leading to the emission of photons of different wavelengths following Planck’s constant. The silicon nanocrystals play a very great role in biomedical engineering. So advancement in the silicon nanocrystal will also advance the biomedical field. Future development can be done by merging nonmetallic ions for recombination.

The cost-effectiveness of the proposed work is of major concern.
Data Availability
The data used to support the findings of this study are included in the article. Should further data or information be required, these are available from the corresponding author upon request.

Conflicts of Interest
The authors declare that there are no conflicts of interest regarding the publication of this paper.

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References


