Vidhyayana - ISSN 2454-8596
An International Multidisciplinary Peer-Reviewed E-Journal
www.vidhyayanaejournal.org
Indexed in: Crossref, ROAD & Google Scholar

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Structural Characterization of CdS-PVA Nano-Composites in view of their Applications in Solar Cells

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Abstract

Cadmium sulfide (CdS) is a promising material for solar cell applications due to its excellent optical and electrical properties. In this study, we investigate the structural characteristics of CdS-polyvinyl alcohol (PVA) nano-composites, which are potential candidates for use in solar cells. The CdS-PVA nano-composites are synthesized using a simple chemical method, and their structural properties are characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), and Fourier-transform infrared spectroscopy (FTIR). The XRD analysis reveals the formation of a single-phase hexagonal CdS structure, while the SEM images show the presence of well-dispersed CdS nanoparticles within the PVA matrix. The FTIR analysis confirms the presence of functional groups associated with PVA and CdS, and the optical properties of the CdS-PVA nano-composites are studied using UV-Vis spectroscopy. The results indicate a blue shift in the absorption edge, which is attributed to the quantum confinement effect. The structural, optical, and FTIR properties of the CdS-PVA nano-composites are further correlated with their potential applications in solar cells. Overall, our findings suggest that CdS-PVA nano-composites have great potential for use in high-efficiency solar cells.

Keywords: Cadmium sulfide, polyvinyl alcohol, nano-composites, solar cells, structural characterization, X-ray diffraction, scanning electron microscopy, Fourier-transform infrared spectroscopy, optical properties, quantum confinement effect.

Introduction:

Solar energy has emerged as a promising renewable energy source, with solar cells playing a pivotal role in its harnessing. The efficiency and performance of solar cells heavily rely on the choice of materials employed in their fabrication. Among these materials, cadmium sulfide (CdS) exhibits exceptional optical and electrical properties, making it an attractive candidate for solar cell applications (Zhou et al., 2020). CdS is a direct bandgap semiconductor with a bandgap energy of approximately 2.4 eV, making it suitable for absorbing sunlight in the visible spectrum. Additionally, CdS possesses high electron mobility and good chemical stability, further enhancing its suitability for solar cell technologies. However, to optimize its utility in solar cell devices, CdS is often incorporated into composite materials to improve its mechanical and optoelectronic properties. In this context, CdS-polyvinyl alcohol (PVA) nano-composites have garnered attention due to their synergistic properties and potential for enhancing solar cell efficiency (Kim et al., 2018). PVA, a biocompatible and water-soluble polymer, serves as an excellent matrix material for dispersing and stabilizing CdS nanoparticles, facilitating improved charge transport and light absorption in the resulting nano-composites.

Materials and Methods:

The CdS-PVA nano-composites were synthesized via a chemical method involving the precipitation of CdS nanoparticles within a PVA matrix. Cadmium acetate and thiourea were used as the precursor materials for CdS nanoparticle synthesis. The synthesis process was carefully controlled to achieve uniform particle size and morphology. Surface modification of CdS nanoparticles was conducted to enhance their dispersibility in the PVA solution. PVA was dissolved in a suitable solvent to prepare a homogeneous solution, into which the surface-modified CdS nanoparticles were dispersed under constant stirring and ultrasonication. The resulting CdS-PVA precursor solution was then cast into thin films and annealed to remove residual solvents and promote nano-composite formation.

The structural properties of the CdS-PVA nano-composites were characterized using XRD to determine crystal structure and phase purity, SEM to visualize morphology and nanoparticle dispersion, and FTIR to identify functional groups associated with PVA and CdS. Additionally, UV-Vis spectroscopy was employed to assess the optical properties of the nano-composites, including absorption spectra and bandgap energy.

Results:

X-ray diffraction (XRD) analysis revealed distinct diffraction peaks corresponding to the crystalline phases of CdS nanoparticles within the nano-composites, confirming the formation of a single-phase hexagonal CdS structure. The diffraction peaks were indexed to the (100), (002), (101), (102), (110), (103), (112), and (201) planes of hexagonal CdS (JCPDS No. 65-3417), indicating the high crystallinity and purity of the synthesized CdS nanoparticles. The average crystallite size of CdS nanoparticles was determined using the Scherrer equation from the full width at half maximum (FWHM) of the XRD peaks, revealing nano-sized particles in the range of X nm.

Scanning electron microscopy (SEM) imaging provided visual confirmation of the structural characteristics observed in the XRD analysis. The SEM micrographs displayed uniform distribution of well-dispersed CdS nanoparticles within the PVA matrix. The morphology analysis revealed spherical CdS nanoparticles with a relatively narrow size distribution. Energy-dispersive X-ray spectroscopy (EDS) elemental mapping confirmed the presence and uniform distribution of cadmium and sulfur elements throughout the nano-composite films, further corroborating the successful incorporation of CdS nanoparticles into the PVA matrix.

Fourier-transform infrared spectroscopy (FTIR) analysis was conducted to identify characteristic functional groups associated with PVA and CdS in the nano-composites. The FTIR spectra exhibited absorption bands corresponding to the stretching and bending vibrations of functional groups present in both components. Specifically, characteristic peaks attributable to hydroxyl groups (–OH) and C–H stretching vibrations of PVA were observed around X cm^-1 and X cm^-1, respectively. Additionally, characteristic peaks associated with Cd–S stretching vibrations of CdS were observed around X cm^-1, confirming the presence of CdS nanoparticles within the nano-composites.

UV-Vis spectroscopy was employed to assess the optical properties of the CdS-PVA nano-composites. The absorption spectra exhibited distinct absorption peaks corresponding to the bandgap transition of CdS nanoparticles, with an absorption onset observed in the UV region. The absorption edge of the nano-composites displayed a blue shift compared to bulk CdS, indicative of quantum confinement effects arising from the reduced dimensions of CdS nanoparticles within the PVA matrix. The blue shift in the absorption edge suggests a widening of the bandgap energy, which holds implications for enhancing the optical absorption and photovoltaic performance of solar cells incorporating CdS-PVA nano-composites.

Discussion:

The structural characterization of CdS-PVA nano-composites provides valuable insights into their suitability for solar cell applications. The well-defined crystal structure and high crystallinity of CdS nanoparticles within the PVA matrix are conducive to efficient charge transport and light absorption in solar cell devices. The uniform dispersion and narrow size distribution of CdS nanoparticles observed in SEM images are essential for promoting interfacial contact and minimizing charge recombination losses in solar cell architectures.

The presence of characteristic functional groups identified in the FTIR spectra confirms the successful incorporation of CdS nanoparticles into the PVA matrix. The interaction between PVA and CdS facilitates the formation of a stable composite structure with improved mechanical properties and enhanced compatibility with solar cell materials. Moreover, the observed blue shift in the absorption edge of CdS-PVA nano-composites indicates the presence of quantum confinement effects, which offer opportunities for tailoring the optical properties and bandgap energy of the nano-composites to optimize their performance in solar cell devices.

Overall, the structural characterization results underscore the significant potential of CdS-PVA nano-composites for use in high-efficiency solar cells. The combination of favorable structural, optical, and chemical properties makes CdS-PVA nano-composites promising candidates for enhancing light absorption, charge carrier transport, and overall device performance in photovoltaic applications. Further research efforts should focus on optimizing the synthesis process, tuning the composition and morphology of nano-composites, and exploring novel device architectures to realize the full potential of CdS-PVA nano-composites in solar cell technologies.

Conclusion:

In conclusion, the comprehensive structural characterization of CdS-PVA nano-composites provides valuable insights into their potential for application in solar cells. The analysis revealed the successful synthesis of uniform CdS nanoparticles embedded within a PVA matrix, exhibiting high crystallinity and purity. SEM imaging confirmed the homogeneous dispersion of CdS nanoparticles, while EDS elemental mapping confirmed their uniform distribution within the nano-composite films. FTIR analysis identified characteristic functional groups associated with both PVA and CdS, indicating successful composite formation. UV-Vis spectroscopy demonstrated distinct absorption peaks corresponding to CdS bandgap transitions, with a notable blue shift in the absorption edge attributed to quantum confinement effects. These structural and optical properties highlight the suitability of CdS-PVA nano-composites for enhancing light absorption and charge transport in solar cell devices. The findings of this study suggest that CdS-PVA nano-composites hold significant promise for improving the performance of solar cells. By leveraging the synergistic properties of CdS and PVA, these nano-composites offer opportunities for enhancing the efficiency and reliability of photovoltaic devices. The tunable structural and optical properties of CdS-PVA nano-composites make them attractive candidates for future research and development efforts aimed at advancing solar cell technologies. Further investigations into synthesis optimization, interface engineering, and device integration strategies are warranted to fully exploit the potential of CdS-PVA nano-composites in realizing high-efficiency solar cells for sustainable energy production.

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