Low Cost Pyrite (Fes₂) Nanorod Sensitized Solar Cell

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Abstract. The fabrication of a low cost, sustainable semiconductor sensitised solar cell is carried out using FeS_2 nanorods as the sensitising material over an electrode coated by TiO_2 nanoparticles. Though the semiconductor sensitised cells are eloquently researched, NR structures as a sensitising material are still not fully investigated despite their features potentially beneficial for accelerating the performance of the devices. The pyrite NR based solar cell is having a notable open circuit voltage of 0.16 V, a short circuit current of 3.9 mA/cm² and an overall conversion efficiency of 0.63%. A simple design and fabrication approach like doctor blading, dip coating is employed throughout the work with an objective to minimise the fabrication cost as much as possible.

Keywords: Pyrite solar cells; FeS₂; nanorods; cheap photovoltaics; photoelctrochemical cell.

1 Introduction

The thin film PV modules photovoltaics market continues to show immense promise these days, but is presently dominated by product based on the use of materials like CdTe, GaAs and silicon wafers, similar to those used in microelectronics. Though the CdTe and GaAs thin film PV modules have the potential to reach cost effective PV-generated electricity, their toxicity and adverse effects on environment drag their feet. The thin film solar cells based on nanomaterials like Dye Sensitised and Semiconductor sensitised solar cells (DSSC) are projected as the most feasible route towards safe, low cost solar cells with decent efficiency. Here we investigate the candidate material Iron pyrite FeS₂, which is an interesting next-generation photovoltaic material that is abundant in nature [1], showing strong absorption[2,3,4] and which is nontoxic as the sensitising material on TiO₂. The highest reported efficiency for a pyrite based solar cell is 2.8% [5]. Interesting photoresponse of FeS₂ deposited polycrystallineTiO₂ electrode using Chemical Vapor deposition method [6] has been reported by Ennaoui et al..Recently Shen et al. [7] have reported the modification of large band gap TiO₂ (Degussa P25) by quantum-sized FeS₂ particles by a similar procedure described by Chatzitheodorou et al. [8]. They reported an incident-photon-to current efficiency of 25% at 400 nm excitation.

Despite various possibilities of the ex-situ assembly route, like sensitizers of different sizes, shapes, and compositions, most efforts in this area are focused on the 0-D semiconductor QDs as sensitizer materials [9,10]. In this work we have sensitised FeS₂ nanorods(NRs) of diameter 12 nm on a TiO₂ layer coated over ITO substrate with I / I_3^- and Pt as the electrolyte and the counter electrodes respective. Throughout this work we have adopted the most simple and cost effective methods for the fabrication of solar cells.

The NR structures open up various possibilities such as band gap tuning by varying the diameter of the NRs along the length [10], orthogonal light absorption and carrier collections directions, minimisation of the recombination of photogenerated carriers by proper channelizing of the carriers [11] in an oriented direction etc., thus reducing the thickness of the absorber layer in such nano-structured solar cells to several hundred nanometers relatively to the traditional thin film solar cells. Also the increased semiconductor surface area in NRs improves the semiconductor-electrolyte interface [11,12,13] and thus creates more photocatalytic reactive sites which is supposed to create better hole transport. The NR structures further show enhanced strain relaxation [14,15] opening up to a broader range of absorption energies than is possible with other planar structures.

2 Materials and Methods

2.1 Materials

ITO glass ($15\Omega/sq$ mm), Platisol, Iodolyte (30 mM iodide/tri-iodide electrolyte) were purchased from solaronix, Switzerland. The FeS₂ NRs were synthesized by a low cost process with FeSO₄ 7H₂O (99 %) and Na₂S₂O₇ (99 %) as Iron and Sulfur sources as reported in our previous work [16], which can be produced on large scale for industrial production. The TiO₂ nanoparticles were synthesized by a similar process as reported in an earlier work with slight modifications [17].

2.2 Materials Characterisation

The X-ray diffraction patterns were recorded by using X-ray diffractometer (XRD, JEOL make, JPX 8) for the identification of phases present in the powder. The morphology and cross section of the electrode were investigated by scanning electron microscope (SEM, JEOL make, JSM-6380LA model). The size of the NRs was determined by TEM (JEOL make, JEM 2100).

2.3 Device Fabrication

The working electrode was prepared by sensitizing pyrite NRs on TiO_2 nanoparticles coated over an ITO substrate (see Supplementary material). Cell assemblies were formed by sealing the counter electrodes which are made by coating a layer of Platisol on an ITO surface to the TiO_2 electrode with Surlyn (DuPont) at 100°C for 1 minute. The corresponding electrolyte was introduced through two small holes, previously drilled through the counter electrode, which were then sealed with Surlyn.

3 Results and Discussion

The efficiency of the FeS₂ NR sensitized cell was calculated by irradiating the cell with active area of 0.54 cm^2 with a light intensity of 100 mW/cm² (AM1.5) and calculating the short-circuit photocurrent density, the open-circuit voltage, the fill factor of the cell. The cell showed an overall efficiency of 0.63% with an open circuit voltage (V_{oc}) of 0.16 V and short circuit current density (J_{sc}) of 3.9 mA /cm². There are several reasons pointed out for the low open circuit voltage in pyrite solar cells. It can be assumed that the major cause of the low open circuit voltage is the ionization of high-density bulk deep donor states [18,19].

These states arise from bulk sulfur vacant sites, which thereby create a varying charge allocation and a very light surface space charge region which reduces the total barrier height and the photovoltage of the pyrite device. The charge carrier transport in these cells can be described only by taking into account the inevitable multistep tunneling via defects in the depletion region, depicting a high density of defects. As further doctor blading is performed successively over the electrode enhancing the thicknesses, the fill factor was almost constant but the short circuit current density and conversion efficiency, were higher (see supplementary material). As mentioned in earlier section the NR morphology of the FeS₂ absorbing layer improved the reduction-oxidation reaction which increased the number of charge carriers and short circuit current density. We can model the NRs as cylindrical wells with infinite barriers which could improve the effective charge transport mechanism. Furthermore, the increase in the doctor blading led to an enhanced loading of the NRs. This could possibly enhance the effective optical path for absorption; due to multiple reflections. The reduced open circuit voltage with more doctor blading can be attributed to the long diffusion distance for the photoelectron to transport to the electrode enhancing the recombination.



Figure 1. (a) TEM image of the TiO₂ NRs (b) diffraction pattern of TiO₂ nanoparticles (c) TEM image of FeS₂ NRs (d) XRD pattern of FeS₂ NRs.



(a)



Figure 2. (a)Side view of Pyrite NR sensitized solar cell (b) SEM cross sectional view of the sensitized electrode (c) Power vs voltage curve (twice successively doctor bladed electrode).

4 Conclusion

We have demonstrated the fabrication and working of a Pyrite sensitised solar cell with a largely unhyped NR structure as the sensitising material. Though the efficiency of the solar cell employing a simple doctorblading approach is low, the cell cannot be underestimated considering the factors like simple design and excellent scope of nanorod structure and pyrite as an absorbing material. We hope this work would seed further research in this area, especially the nanorod morphology as a possible absorbing material.

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References

- 1. A. Ennaoui, H. Tributsch, Iron sulphide solar cells, Sol. Energ. Mat. Sol. C. 13(2), 197-200 (1984).
- T. Hong, Low-temperature synthesis of size-controllable anatase TiO₂ microspheres and interface optimization of bi-layer anodes for high efficiency dye sensitized solar cells, Electrochim. Acta. 137, 17-25 (2014).
- J.M. Lucas, C.C. Tuan, D.L. Sebastien, K.B. David, R. Qiao, W. Yang, A. Lanzara, A.P. Alivisatos, Ligandcontrolled colloidal synthesis and electronic structure characterization of cubic iron pyrite (FeS₂) nanocrystals, Chem. Mater. 25, 1615-1620 (2013).
- 4. Y. Bai, J. Yeom, M. Yang, S.H. Cha, K. Sun, and A.N. Kotov, J. Phys. Chem. C 117, 62567-2573 (2013).
- A. Ennaoui, S. Fiechter, G. Smestad and H. Tributsch, Proc. 1st World Renewable Energy Congress, Reading, UK, Pergamon Press, City pp. 458 1990.
- T. Dittrich, A. Belaidi, A. Ennaoui, Concepts of inorganic solid-state nanostructured solar cells, Sol. Energ. Mater. Sol. C. vol. 95, 1527-1536 (2011).
- Y. C. Shen, H. Deng, J. Fang, and Z. Lu, Co-sensitization of microporous TiO₂ electrodes with dye molecules and quantum-sized semiconductor particles, Colloid. Surface. A 175, 135–140 (2000).
- G. Chatzitheodorou, S. Fiechter, M. Kunst, J. Luck, and H.Tributsch, Low temperature chemical preparation of semiconducting transition metal chalcogenide films for energy conversion and storage, lubrication and surface protection, Mater. Res. Bull. 23, 1261-1271 (2003).

- N. Guijarro, J.M. Campina, Q. Shen, T. Toyoda, T. Lana-Villarreala, R. Gómez, Uncovering the Role of the ZnS Treatment in the Performance of Quantum Dot Sensitized Solar Cells, Phys. Chem. Chem. Phys. 13, 12024– 12032 (2011).
- J.T Margraf, A. Ruland, V. Sgobba, D.M. Guldi, T. Clark, Quantum-Dot-Sensitized Solar Cells: Understanding Linker Molecules through Theory and Experiment, Langmuir 29, 2434–2438 (2013).
- H. McDaniel, N. Fuke, N.S. Makarov, J.M. Pietryga, V.I. Klimov, An Integrated Approach to Realizing High-Performance Liquid-Junction Quantum Dot Sensitized Solar Cells, Nat. Commun. 4, 2887-2896 (2013).
- K. Sunita, K. Simanta, P. Amitava, K.G. Ashok, Band gap tuning of ZnO/In₂S₃ core/shell nanorod arrays for enhanced visible-light-driven photocatalysis, J. Phys. Chem. C 117, 5558-5567 (2013).
- M.S. Eichfeld, Synthesis and characterization of silicon nanowire arrays for photovoltaic applications. Diss. The Pennsylvania State University 2009.
- Y.H.J. Lee, Z. Li, L. Fu, P. Parkinson, K. Vora, H.H. Tan, C. Jagadish, Improved GaAs nanowire solar cells using AlGaAs for surface passivation, Optoelectronic and Microelectronic Materials & Devices, Proceedings, COMMAD 131-132 (2012).
- J. Bai, Q. Wang, T. Wang, Characterization of InGaN-based nanorod light emitting diodes with different indium compositions, J. Appl. Phys. 111, 113103(2012).
- P. Namanu, M. Jayalakshmi, K. Udayabhat, Low temperature synthesis of Iron pyrite nanorods for photovoltaic applications, J. Mater. Sci: Mater. Electron. 26, 8534-8539 (2015).
- M.M. Ba-Abbad, A.A.H. Kadhum, A.B. Mohamad, M.S. Takriff, K. Sopian, Int. J. Electrochem. Sci. 7, 4871-4888 (2012).
- S. Ruoshi, M.K.Y. Chan, G. Ceder, First-principles electronic structure and relative stability of pyrite and marcasite: Implications for photovoltaic performance, Phys. Rev. B 83, 235311 (2011).
- A. Krishnamoorthy, F.W. Herbert , S. Yip, K.J. Van Vliet , B. Yildiz, Electronic states of intrinsic surface and bulk vacancies in FeS₂, J. Phys. Condens. Matter. 25, 045004 (2012).