

Effect of varying reactant precursors on synthesis of nanostructured Iron disulphide (FeS₂)

Gurpreet Kaur¹, Bikramjeet Singh¹, Paviter Singh¹, Manpreet Kaur¹, Anup Thakur², Manjeet Kumar³, Rajni Bala⁴, Akshay Kumar^{1*}

¹Department of Nanotechnology, Advanced Functional Material Laboratory, Sri Guru Granth Sahib World University, Fatehgarh Sahib, Punjab 140406, India

²Department of Basic and Applied Sciences, Punjabi University, Patiala, Punjab 147002, India

³Department of Materials Engineering, Institute of Advanced Technology (DU), Pune 411025, India

⁴Department of Mathematics, Punjabi University, Patiala, Punjab 147002, India

*Corresponding author, Tel: (+91) 9592778910; E-mail: akshaykumar.tiet@gmail.com

Received: 30 March 2016, Revised: 29 September 2016 and Accepted: 21 December 2016

DOI: 10.5185/amp.2017/211

www.vbripress.com/amp

Abstract

Nontoxic and earth abundant nanostructured semiconductors have experienced wide attention of researchers recently. One of the more studied material is Iron pyrite (FeS₂) owing many different promising applications. Herein, the synthesis of nanostructures by varying the reactant precursors of iron and sulphur has been reported. The molar ratio of iron and sulphur precursors play a crucial role in determining the quality of nanostructures. This work further advances synthesis with pyrite purity, structure control and then promotes use in photovoltaics, photocatalysis and photoelectrochemistry applications. Copyright © 2017 VBRI Press.

Keywords: Iron disulphide, photovoltaics, photocatalysis, reactant precursors.

Introduction

Pyrite (FeS₂) is one of natural most earth abundant material and is cheap in cost. Pyrite has gained centre of attraction for researchers due to its high absorption coefficient ($\sim 10^5 \text{ cm}^{-1}$) and low energy band gap with a direct transition ($\sim 0.9 \text{ eV}$) [1-3]. Till date, many researchers have evaluated CdTe, CuInGaSe₂ (CIGS), and Si, for solar cell applications. On the contrast, Selenium, Gallium, Tellurium and Indium all are rare earth materials and also expensive in cost [4-5]. The material for photovoltaic applications should be earth abundant, cheap and have high performance properties. The pyrite becomes very attractive material for next generation photovoltaic applications. The formation mechanism of FeS₂ play a vital role to improve the surface stability and control the impurity phases.

In this study, FeS₂ nanostructures were synthesized using hydrothermal method. As hydrothermal method has some benefits such as high yield, pure products and suitable for mass production. The molar ratio of sulphur to iron precursors play an important role in formation of single phase FeS₂ nanostructures.

Experimental

Materials

Iron (II) chloride tetrahydrate (FeCl₂.4H₂O, Aldrich 99%) and Sodium thiosulfate (Na₂S₂O₃.5H₂O, Aldrich 98%) were used as the precursor materials, and the mole ratio of Fe:S was kept to 1:4. The structural properties of iron disulfide nanostructures were examined by X-ray diffraction (XRD, PANalytical).

Methods

The iron disulfide nanostructures were synthesized using hydrothermal method. Iron (II) chloride tetrahydrate (FeCl₂.4H₂O) and Sodium thiosulfate (Na₂S₂O₃.5H₂O) were used as the precursor materials, and the mole ratio of Fe:S kept to change as 1:4, 1:3, 1:2 respectively. The aqueous solutions of both precursors iron and sulphur were mixed homogeneously using magnetic stirring. After obtaining a homogeneous mixture, the solution was transferred to a Teflon lined stainless steel at 180°C for 12 hours.

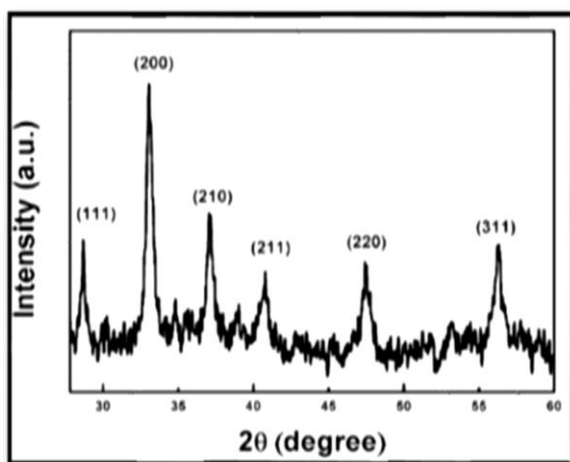


Fig. 1. XRD pattern of FeS₂ nanostructures synthesized with [S]/[Fe] 4:1.

Results and discussion

The crystal structures are examined by XRD patterns as shown in Fig. 1, 2 and 3. The diffraction peaks associated with pyrite FeS₂ are observed and indexed as a pure cubic phase of FeS₂ (space group P1 (1) with a lattice constant of 5.417 Å), which is consistent with the value given in the standard card (JCPDS no. 65-1211).

Pyrite (FeS₂) becomes the governing material when there is increase in sulphur concentration with respect to iron precursor concentration as the intensity of iron oxide peaks drops dramatically. The formation of S²⁻ results as excess sulphur is necessary to drive the reaction processes due to less reactive nature of sulphur as compared to Fe²⁺. The impurities are significantly reduced and nearly disappear in XRD pattern (Fig. 1).

When sulphur to iron precursor concentration varies as 3:1, XRD pattern indicates the number of phases are reduced as the sulphur excess is used for synthesis (Fig. 2). In Fig. 3, XRD pattern revealed the impurity phases are observed such as troilite (ICDD 001-1247), Pyrrhotite (017- 0201), Marcasite (002-1342) and Haematite (024-0072) as synthesis method involve the use of aqueous medium.

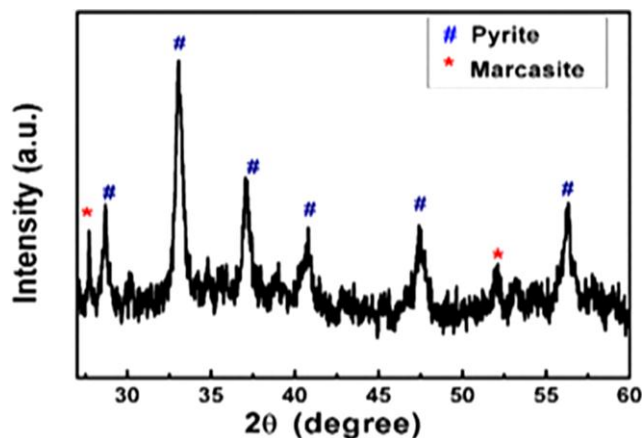


Fig. 2. XRD pattern of as obtained sample Iron disulphide when [S]/[Fe] is 3:1.

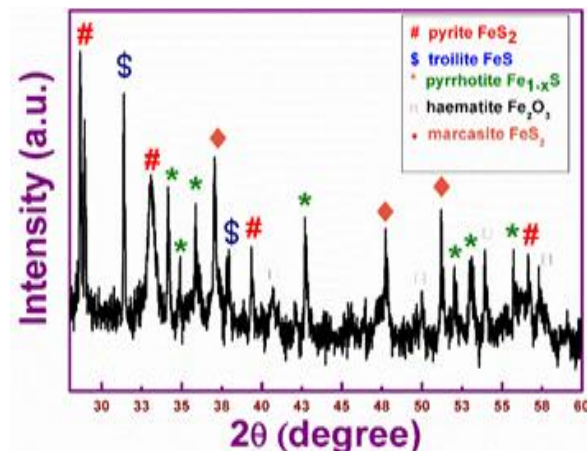


Fig. 3. XRD pattern of as obtained sample Iron disulphide when [S]/[Fe] is 2:1.

Conclusion

Iron disulphide (pyrite) nanostructures were synthesized using a simple synthesis route. The impurity phases such as troilite and marcasite can be reduced efficiently by adding excess sulphur and thus leads to a single phase iron disulphide nanostructures. The iron disulphide single phase nanostructures may find their applications in field of photovoltaics and rechargeable batteries.

Acknowledgements

This work was supported by Minority fellowship for Maulana Azad National Fellowship (file number - 36753) (MANF Program) from Department of Minority Affairs India (Moma).

Author's contributions

Conceived the plan: Akshay Kumar; Performed the experiments: Gurpreet Kaur, Bikramjeet Singh, Paviter Singh, Manpreet Kaur; Data analysis: Manjeet Kumar, Rajni Bala; Wrote the paper: Akshay Kumar, Anup Thakur.

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