Summary

Title of the Research Project: **'Studies on $Cd_{1-x}Fe_xS$ Thin Films: Prospectus in Solar Cell'**

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In recent years, there has been considerable interest in the field of photoelectrochemical cell, because of its potential application in solar energy conversion and utilization. For enhancing the efficiency of light conversion, it is most important to develop semiconductors with suitable band gap. For a PEC solar cell, the prime requirement for good solar energy conversion is that the photoanode/ photocathode should have a bandgap close to the maximum in the visible spectrum to utilize the solar spectrum efficiently; second, the semiconductor electrodes must be stable against photocathodic/photoanodic reactions. These cells are simple in construction and have the advantage that they can be used for both solar to electrical and chemical energy conversions. Presently, one of the best materials where tailoring of bandgap is possible is from the group of Cd-chalcogenides. Binary semiconductors of II-VI group attracts many researchers, because of their wide range of applications in solid state devices, such as solar cells, opto-electronic devices, solar selective coatings. In recent years, many important physical properties of Fe based II–VI semiconductor materials were studied in theory and experiment, such as $Cd_{1-x}Fe_x$ S, $Cd_{1-x}Fe_xTe$, $Cd_{1-x}Fe_x$ Se, $Zn_{1-x}Fe_x$ Se, and $Zn_{1-x}Fe_x$ S. Among II-VI group semiconductors, CdS is an important material which has been mainly utilized for photoelectrochemical solar cells, opto-electronic devices, piezoelectric transducers and window layers in heterojunction solar cells, etc. CdS is found to be an excellent material with a direct band gap value of 2.42 eV which make them interesting for photoelectrochemical solar cells, because of their compatibility of its bandgap with the solar spectrum. Incorporation of Fe ions is expected to bring some novel properties related to spintronics while keeping the outstanding properties of CdS. Among different DMS hosts that have been investigated, transition metal doped

CdS, in particular, Fe doped CdS has gained substantial interest due to the existence of spin-orbit interaction and large exchange interaction.

We have therefore selected a cadmium-cobalt-sulphide ternary system because : 1) cadmium sulfide and ferrous sulfide have direct band gaps and high coefficients of optical absorption and excellent stability, 2) the bandgap of pure CdS can be tailored by the incorporation of Fe in CdS and can be made to match with the VIS/NIR regions of the electromagnetic spectrum, 3) Both CdS and FeS are identical in structure and therefore a large Fe-content can be accommodated in the lattice of CdS, 4) Both have extremely narrow single phase region and a moderate negative free energy of formation that facilitate the deposition of these materials over a wide range of the preparative conditions and 5) CdS and $Cd_{1-x}Fe_xS$ are stable and can be prepared by an universal (extremely simple and inexpensive) chemical growth process. Therefore, it is expected that CdS and Fe may form a solid solution over a large range of their miscibilities thus allowing the bandgap to vary between two energy gap limits of the semiconductors. This can be achieved simply by changing the molar composition, x. A quality solar material must have: i) high sensitivity, ii) high quantum conversion efficiency, iii) broad spectral response in the range of operating wavelengths, iv) low dark current (reverse leakage) and v) low signal dependent noise. Additionally, the responsivity depends on the bandgap of the material, operating wavelengths, doping concentration and thickness of the material. Keeping this idea into mind and considering our laboratory and experimental limits, systematic studies, were planned to fabricate and characterize the CdS and $Cd_{1-x}Fe_xS$ solid solution thin films and to employ them as an electrode in photovoltaic solar cells. The work was carried out through various successive linked stages such as deposition of the thin films, characterization, analysis and their application in PV solar cells and their characterization. A chemical deposition route was followed for the deposition purpose. This technique works on the principle of an ion-by-ion condensation and is capable of producing uniform and homogeneous layers of controlled composition. The preparative parameters can be easily controlled and will be finalized in the initial stages of the work. The kinetics of growth mechanism will be examined. The film structures will then be determined through their structural and microscopic observations. The optical and electrical transport characteristics and various film parameters were studied. The $Cd_{1-x}Fe_xS$ film structures will also be obtained on the conducting substrates and a best match of an electrolyte will be searched out by fabricating the electrochemical-PV systems. These systems will then be characterized through the electrical characteristics and optical properties. Having been understood the basics of a chemical bath deposition technique and the potential applicability of $Cd_{1-x}Fe_xS$ based PV-cells, we propose to develop (Cd, Fe)S semiconductor films of excellent structure, morphology and characteristics within the experimental limits of our Thin Film & Solar Studies Research (TF & SSR) Laboratory.

In the proposed work we have planned for a multistep research program and the actual quanta of the work carried out as follows

Begins with the general introduction of the subject and need of the Solar Energy have been discussed. An exhaustive survey of literature and current status of CdS and CdFeS thin films have also been described. The experimental techniques used to characterize CdS and CdFeS thin films. The proposed work of project focuses on the preparation of CdS and CdFeS thin films by a liquid phase chemical bath deposition method. Growth mechanism, reaction kinetics, wettability measurements and a detailed account of the materials composition, structural, spectroscopic and microscopic observations, optical and electrical transport properties on these films are described in details. The various preparative parameters like deposition temperature, time, pH of the reaction mixture and speed of the substrate rotation can easily be manipulated and optimized to obtain good quality deposition of the films. Thin, relatively uniform, smooth, physically adherent and diffusely reflecting films can be obtained using CBD. The polycrystalline growth of CdS and CdFeS thin films is made feasible and the deposits exhibit hexagonal wurtzite structure. The grain sizes are of the order of few nm. Optical band gap of the $Cd_{1-x}Fe_xS$ thin films can be tuned as desired. The thermoelectric power is of the order of few micro volts and samples showed n-type conduction. Finally we have successfully synthesis CdS, CdFeS thin films (on stainless substrates) for PV applications.

The present work is communicated and some work has been published in Seminar Proceeding.

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