Suitability of Materials for Photovoltaics

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Abstract:-Materials play a key role in various aspects of solar energy conversion. Presently available materials are generally deficient in performance, cost, stability or some combination thereof. New material systems, guided by the interplay between rational design, high-throughout screening and theory, are needed to improve the performance of light absorbers, photovoltaic materials and photo-electrodes. The catalysts, thermo-electrics and infrastructural aspects of solar energy conversion systems need further improvement. Polymer solar cells and dye selenized solar cells are being studied now-a-days with great interest all over the world because they have the great potential for the future. The introduction of nanotechnology also has raised a lot of expectations.

Introduction:- Materials play a key role in solar energy conversion to electricity, fuels and heat. Materials used in photovoltaics have traditionally been derived from research and development advances in other technological fields (e.g. Si from microelectronics industry, GaAs from optoelectronics industry) and as a result, the range of materials currently available for use in photovoltaics is highly limited compared to the enromous number of semiconductor materials that can (in principle) be synthesized for use in photovoltaics.[1]. Similarly, high-efficiency thermoelectric and thermophotovoltaic converters coupled to solar concentrators have the potential to generate electricity at converter efficiencies upto 35% and more. Significant progress has been made in these areas over the last two decades, particularly by exploiting nanoscience and nanotechnology. Further fundamental research can lead to cost effective materials that enable efficient solar-thermal energy utilization systems. Solar concentrators and hot water heaters call for new lowcost polymer-based materials/ composites, while new solar thermal storage materials are required for several solar thermal conversion applications.

Determining the suitability of materials for photovoltaics is currently not a systematic process. For example, one of the most widely used semiconductors for thin film photovoltaic cells is copper-indium-gallium-diselendie ($Cu_xGa_{1-x}InSe_2$). It was unexpectedly discovered that small area $Cu_xGa_{1-x}InSe_2$ cells work very well, despite being polycrystalline and containing many point defects, because sodium diffuses from glass substrates into the $Cu_xGa_{1-x}InSe_2$ film, interacts with grain boundaries and reduces recombination. If the initially undesired sodium diffusion had not occurred, it is not clear that $Cu_xGa_{1-x}InSe_2$ technology would have reached its current state of development. This example points out the importance of experimentally testing films with many combinations of elements, even if there is no underlying heuristic or formal theoretical prediction suggesting that such combinations might have desirable properties. Since there are enormous numbers of alloy compositions to try, high-throughput screening methods are needed.

Furthermore, promising polycrystalline thin film solar cells based on CdTe and $CuInSe_2$ are dramatically affected by the grain structure resulting from growth on foreign substrates, intentional and/or unintentional doping by impurities, the nature of the active junction and ohmic contacts; all these processes and effects are poorly understood. A basic understanding of these issues would facilitate a revolutionary advance in the performance and economic viability of polycrystalline thin film PV.

High Throughput Experimental Screening Methods for Discovery of Designed Materials: A big research challenged here is to find appropriate and efficient tests of specific photovoltaic properties that enable testing for millions of material combinations. Often materials synthesis is not itself the bottleneck in an approach, owing to relatively straightforward vapor deposition methods for multiple source deposition of elements to form compounds, the more difficult challenge is to develop experimental methods for propertiesbased materials selection. As an example, the energy band gap of the materials could quickly be determined by measuring the absorption spectrum. Some information on the rate at which recombination occurs could be determined by measuring the photoluminescence efficiency. Conceivably, arrays of solar cells could be made to directly determine quantum efficiency, fill factor and open circuit voltage. In this case, contact-less methods for properties measurements would be highly desirable and Pump probespectroscopic techniques could be used to determine the cross-section for impact ionization (multiple electron-hole pair generation). Ideally, such screening methods will identify good candidates for more thorough photovoltaic testing.

Nano-engineered bulk materials my indeed be a key to achieving high performance bulk thermoelectric materials. Understanding the role and stability of the interface between the nano-materials and the matrix is essential in order to effectively optimize the materials. An effective interface must be thermally stable and promote electron transport while impeding phonon transport. Interface issues such as diffusion and segregation processes, doping and composition of the nanostructure, differential thermal expansion and chemical contrast are essential for investigation.

It has been demonstrated experimentally that the phonon thermal conductivity of super lattices can be significantly smaller than the theoretical minima of their constituent bulk materials [3]. Modeling suggests that it is the incoherent superposition of interface reflection of phonon that is the major cause of phonon thermal conductivity reduction [1,2].

We gain a basic uderstanding of novel materials for spectal control from Fleming et al [5] and Greffet et al.[6]. Photonic crystals, plasmonics, phonon polaritons, coherent thermal emission, left handed materials and doping with lanthanides are concepts from the optics community that can be exploited for the spectral control components required in TPV systems. The lanthanides, due to the suitability of their discrete energy levels for photon conversion inside, has attracted a number of researchers [7].

Heat transfer surfaces for water heaters call for polymer/composites with high mechanical strength, UV degradation resistance, high thermal conductivity and concentrator support structures requiring polymers with high mechanical strength and a low thermal expansion coefficient.

The thermal conductivity of most polymers. is 0.2 to 0.4 W/m-K. An order-of magnitude increase in thermal conductivity is needed to make polymers competitive. Now composite materials hold the promise of high mechanical strength the high thermal conductivity. Surface modifications are needed for photon and thermal management. Mirrors and glass that are dirt replelling can significantly increase efficiency and reduce clearing cost. Surface engineering is also needed to prevent scale formation in solar thermal heat exchangers. Fundamental research on particle-surface interactions and solid precipitation and deposition processes can help solve these challenges.

Thermal storage materials must have high latent heat density (>0.3 MJ/Kg.) and sufficiently high thermal conductivity for enhanced thermal energy charge/ discharge processes Recent development of nanocrystal polymer composites can be the key to a stable cycling solution for thermal storage. The unique characteristics of solid solid structural transformations in nanocrystals can lead to a new generation of thermal storage materials. Present thermal storage materials are limited by the lack of reversibility of structural transformations in extended solids. In contrast, nanocrystals embedded in a “soft matrix” can reversibility undergo structural transitions involving a large volume change per unit cell. This is because a structural transition in a nanocrystal may proceed through a single nucleation event per particle (Figure). Further, a nanocrystal can change shape and volume without undergoing fracture or plastic deformation. In addition, the barrier to a structural transition depends strongly on the size of the nanocrystals so that the hysteresis and kinetics of the structural transition can be controlled.

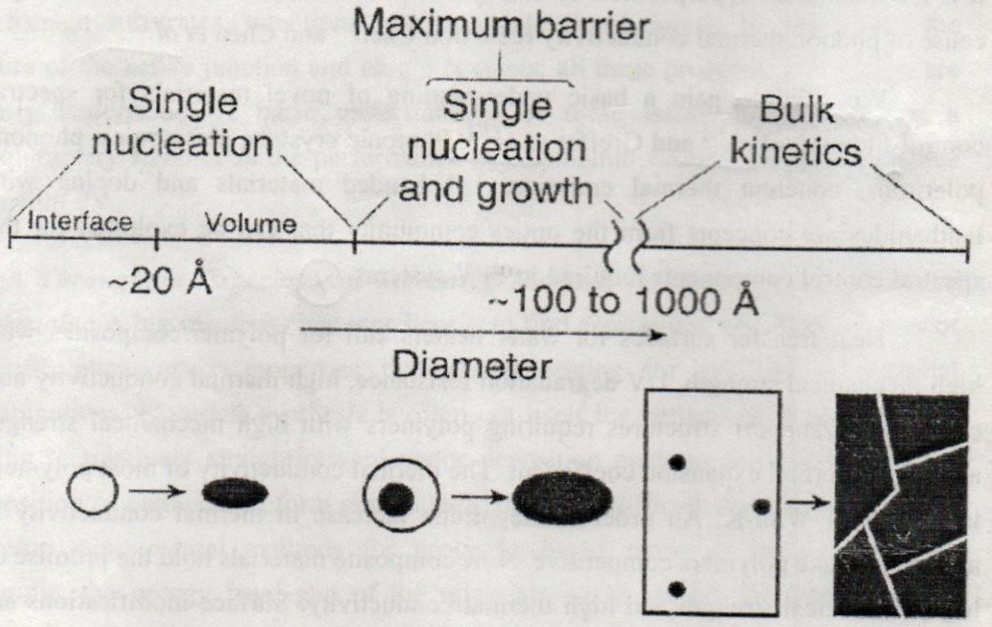

Figure : **Illustration of Various Size Regimes of the Kinetics of Solid-Solid Phase Transitions. Defects, which Act as Nucleation Sites, are Indicated by Round Marks in the Cartoon of the Bulk Solid.**

Potential Impacts and Conclusion: An investment in Research and Development of basic science and technology targeting solar-related materials is extremely relevant to the efficiency and cost goals in the solar energy area. Although there are several materials available to make thin film PV cells today, including SnS [8], an ideal material has not yet been found. Experimental and theoretical screening could discover several direct band gap semiconductors that have band gaps ranging from 0.7 eV-2.5eV, which may function well in PV cells and are made from elements abundant in the Earth's crust. New materials could lead to the development of devices that enable the achievement of an highly efficient power conversion in concentrated solar systems.

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