

Ordered polycrystalline thin films for high performance CdTe/CdS solar cells

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Abstract

An ordered polycrystalline approach is proposed to overcome fundamental problems associated with random polycrystalline thin films, namely grain boundaries and inhomogeneity. The approach consists of two main steps: (1) the deposition of a patterned growth mask and (2) the selective-area deposition of the ordered polycrystals. The ordered polycrystalline approach was investigated using the CdTe/CdS material system. Experimental results demonstrate that SiO₂ and Si₃N₄ are effective growth masks and that temperature is a dominant parameter for selective-area deposition. PL and XRD characterization indicates that the ordered polycrystalline technique has the potential for improving the crystal quality and order of polycrystalline CdTe thin films. The approach appears to be fairly general and could be applied to other material systems.

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1. Introduction

CdTe is a good absorber layer for solar cells with a predicted efficiency of 29% due to its near optimal direct bandgap of 1.45 eV and large optical absorption ($>10^4$ cm⁻¹) above the bandgap [1,2]. This promise has generated much research interest in low-cost thin film polycrystalline CdTe/CdS photovoltaic modules. Although steady improvement in conversion efficiency was achieved in the late 1980s and early 1990s, Fig. 1 shows that the highest reported efficiency has remained essentially flat at 16–16.5% for the last 11 years despite a high degree of research effort [3]. Due to the difficulty of performing scientific study on random polycrystalline semiconductors, much of the research has utilized an empirical approach with narrow applicability and this has hampered fundamental understanding. Studies have isolated and quantified

major issues associated with processing and cell structure [4,5] however consensus is now building that the random nature of polycrystalline films is the fundamental reason preventing technological advancement and deep scientific understanding [2].

The randomness of polycrystalline films has hampered technological development and scientific study in at least two ways. First, the grain boundaries create interdependencies between processing steps and critical device parameters that make isolated study and development difficult [6]. Grain boundaries give rise to a host of issues including: (a) enhanced migration of dopants [5,6], (b) device shunting [7], and (c) high recombination velocities due to unpassivated surfaces. Because grain boundaries form an interconnected network within the thin film, they couple critical components of the device including the back contact, CdTe grains, and the CdS/CdTe junction. For example, isolated study and development of the back contact are nearly impossible due to the effect that back-end processing will have on the doping of CdTe and the CdTe/CdS interface [8]. Moreover, the enhanced migration of copper through

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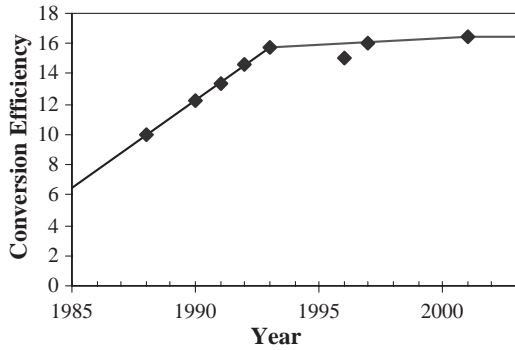


Fig. 1. Highest reported CdS/CdTe solar cell conversion efficiencies from the year 1985 to 2004.

grain boundaries has also been associated with device instability [9]. The need therefore exists to decouple the various processing steps so that significant scientific understanding and technological development can be achieved.

Second, it is well known that inhomogeneity in cell electrical characteristics results in increased losses [10]. Nonuniformity is highly detrimental for two reasons. One is that the optimum performance of each granular cell is not achieved. The second and more insidious reason is that poor performing cells become electrical loads to good cells. Doping and structure engineering in semiconductors are the principal methods to tailor device characteristics. This is also true in solar cells where the doping profile, bandgap and layer thicknesses have dominant effects on cell characteristics. However, controlling the doping profile and structure uniformly in polycrystalline thin films is difficult due to the random nature of the grains and grain boundaries which prevents the desired optimum CdS/CdTe structure and doping from being achieved. The best that can be achieved is an average profile and structure with some degree of statistical nonuniformity. Fig. 2 shows that although the average grain size of CdTe can be controlled by lowering the deposition temperature from 625 °C to 575 °C, close inspection reveals that the film remains random.

The combination of grain boundary effects and the random nature of common processes create a situation that significantly complicates scientific study and technological development. As a result, a plethora of empirical research has yielded only a limited understanding of important

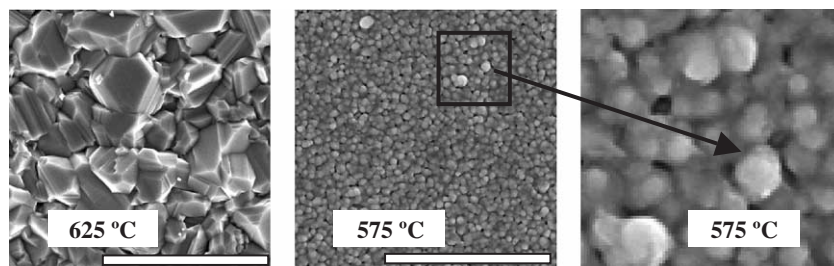


Fig. 2. Effect of deposition temperature on uniformity of CdTe deposited on CdS. Although the uniformity is improved when the temperature is lowered, the image on the far right shows that traditional techniques result in inherently random shaped and oriented crystal grains. The scale bar indicates 22.5 μm.

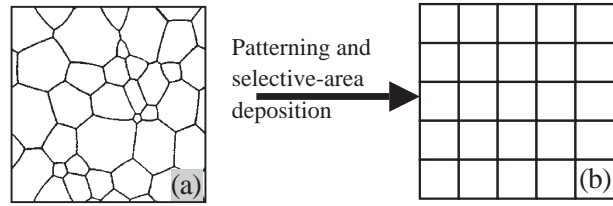


Fig. 3. Basic concept of ordered polycrystalline arrays in comparison to random polycrystalline thin films; in (a) the crystal sizes and shapes of films obtained from conventional deposition processes are random, in (b) patterning and selective-area deposition is utilized to obtain crystals with ordered crystal grains and boundaries.

relationships between processing conditions, structure and device characteristics. For example, the CdCl₂ treatment is known to be very important to dopant activation and grain growth and many recipes have been developed, however the fundamental mechanism is not well understood [1].

Work in the late 70s on single crystal CdTe/CdS solar cells resulted in significant progress. Cells prepared by epitaxial growth of CdS on p-type single crystal CdTe exhibited a conversion efficiency of 11.7% [11]. However, a significant challenge was the high density of defects due to the lattice (~ 10%) and thermal mismatch between CdS and CdTe. Much of the effort has focused instead in polycrystalline processes due to their promise for creating an acceptable tradeoff between efficiency and low-cost manufacturing [12].

Although relatively little work has been done on single crystal CdS/CdTe for solar cell applications, a large amount of work has focused on integrating a wide variety of lattice-mismatched material systems for advanced device applications. For over three decades, high quality crystal growth has been studied to create complex semiconductor structures and to integrate heterogeneous materials for the purpose of increasing device performance and system functionality. As a result, epitaxy has evolved from homoepitaxy to lattice-mismatched heteroepitaxy and from planar growth to patterned epitaxy. Patterned selective-area growth of lattice-mismatched semiconductors has been effectively utilized in a number of material systems to reduce defects and enhance performance [13,14]. For example, Fitzgerald et al. showed a reduction in defects in patterned GaAs grown on Silicon [15] and Zubia et al. showed three-dimensional relief mechanisms at the nanos-

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