NATIVE AND LIGHT INDUCED DEFECT STATES IN WIDE BAND GAP HYDROGENATED AMORPHOUS SILICON-CARBON(a-Si$_{1-x}$ C$_x$:H) ALLOY THIN FILMS

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1. Abstract

In this study, wide band gap a-Si$_{1-x}$ C$_x$:H alloy thin films prepared with and without hydrogen dilution of (SiH$_4$ +CH$_4$) were characterized using optical absorption, dark conductivity, steady-state photoconductivity, sub-bandgap absorption obtained with both photothermal deflection spectroscopy (PDS) and dual beam photoconductivity (DBP), and electron spin resonance (ESR) techniques. Experimental results of steady-state photoconductivity and sub-bandgap absorption for different generation rates were analyzed using a detailed numerical model based on Simmons-Taylor statistics. The densities, energy location and nature of the native and light induced defect states in diluted and undiluted a-Si$_{1-x}$ C$_x$:H alloy thin films were derived from the best fits to the experimental data. The extracted parameters for defect states were compared with those of a-Si:H films both in the annealed and light degraded states.

2. Introduction

High quality, wide band gap hydrogenated amorphous silicon-carbon (a-Si$_{1-x}$ C$_x$:H) alloy thin films are desired for use as an intrinsic layer in the top cell of multijuntion solar cells[1] and as p-type layers of these and other electronic devices. It is well known that these materials can be prepared using glow discharge decomposition of silane and hydrocarbons such as methane(CH$_4$) [2,-5] or using sputtering techniques [5]. However, these wide band gap a-Si$_{1-x}$ C$_x$:H alloy materials were not so photosensitive. As the concentration of carbon in the film increases, dark and photoconductivity decrease, the density of localized defect states increases so do the optical gap and inverse slope of valence band tails, E$_{ov}$ [2-6]. Alternatively, it was reported that the wide band gap a-Si$_{1-x}$ C$_x$:H alloys prepared using H$_2$ -dilution of (SiH$_4$ +CH$_4$) gas mixture significantly improved the optoelectronic properties [7]. Later, this was supported by the studies of Baker et al.[8] and Li et al[9], who also reported that hydrogen dilution improved both dark and photoconductivity by several orders of magnitude. Recently, Lu et al. carried out more detailed studies on the process-property relations of a-Si$_{1-x}$ C$_x$:H alloys deposited in PECVD system as a function of H$_2$ -dilution ratio [10,11]. They reported that an increase in H$_2$ -dilution resulted in an increase in surface smoothening, an increase in

the electron $\mu\tau$ products, and a decrease in the sub-bandgap absorption, a decrease in the inverse slope of valence band tails, E_{ov}, and a decrease in the void fraction. They obtained optimum optoelectronic and microstructural properties of a-$Si_{1-x}C_x$:H alloys for dilution ratios of 20 to 24. Moreover, p-i-n homojunction solar cells prepared using diluted undoped a-$Si_{1-x}C_x$:H alloy layers showed high open-circuit voltages(V_{oc}) and high fill factors [9].

Even though there were improvements in the optoelectronic properties, the defect states in a-$Si_{1-x}C_x$:H alloy thin films have not been studied and well characterized as extensively as those in a-Si:H thin films. Generally, electron spin resonance (ESR) [5], constant photo current method (CPM) [12], and photothermal deflection spectroscopy (PDS) [6,8,9] have been used. The density of defect states were derived either from the integration of CPM and PDS spectrum using the same integration constants, which were derived for a-Si:H thin films not for a-$Si_{1-x}C_x$:H alloys, or directly from ESR spins [3,5]. Due to higher density of surface/interface defect states, both ESR and PDS cannot be used for a reliable characterization of the bulk native defects in the annealed state. Alternatively, an approach of deconvolution of PDS and CPM spectrum was also used to obtain the distribution of defect states in the band gap[13]. However, this method ignores conduction band tails and does not take into account the presence of different defect states with different nature.

In addition, wide band gap a-$Si_{1-x}C_x$:H alloys also have intrinsic property of light induced degradation known as the Staebler-Wronski effect[14]. This has not been studied in detail yet and it is essential to determine long term stability of a-$Si_{1-x}C_x$:H based solar cells. Therefore, detailed characterizations of native and light induced defect states are necessary to understand the origins of these defects and mechanism for the Staebler-Wronski effect in wide band gap a-$Si_{1-x}C_x$:H alloys.

In this paper, wide band gap hydrogenated amorphous silicon-carbon alloy thin films prepared with and without H_2-dilution of (SiH4 + CH4) were studied using optical spectroscopy, dark and photo conductivity, and sub-bangap absorption obtained with dual beam photoconductivity (DBP) technique[15] both in the annealed and light degraded states. The experimental results of photoconductivity and sub-bandgap absorption spectra were analyzed using a detailed numerical model described elsewhere[16].

3. Experimental Details

Steady-state photoconductivity and sub-bandgap absorption measurements were carried out on around 1 μm thick undoped a-$Si_{1-x}C_x$:H alloy thin films deposited on 7059 glass substrate. Deposition conditions for these films were discussed elsewhere[9-11]. Optical absorption in the visible region of the spectrum was obtained from the transmission(T) and reflection(R) measurements and used to normalize sub-bandgap photoconductivities. The optical gaps were derived from the Tauc relation[17]. The ESR measurements were carried out on films codeposited onto quartz substrates. The annealed state was obtained by heating the samples at 200 °C for 12h in N_2 ambient and stabilized light soaked state was obtained by illuminating through both sides of the samples for more than 300h with 1W/cm² white light from an ELH light source filtered with both an IR reflector and IR absorber. Light soaking