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Carrier transport property in the amorphous silicon/amorphous silicon carbide multilayer studied by the transient grating technique

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The in-plane diffusion coefficient and lifetime of photogenerated carriers in amorphous silicon have been measured by the transient grating technique in amorphous silicon (a-Si)/silicon carbide (a-SiC) multilayered structures, as a function of the a-Si well layer thickness. As the layer thickness is decreased, the diffusion coefficient gradually decreases, while the lifetime drastically increases by more than one order of magnitude than that in thick unlayered a-Si. These behaviors suggest that the carrier transport is determined both by carrier interaction with shallow traps at a-Si/a-SiC interfaces and by quantum-size effect through weakened carrier coupling with deep states.

Amorphous semiconductor multilayered structures exhibit several peculiar features, some of which are indicative of the presence of quantum-size effects although not so clear as compared in the case of crystalline superlattices. The effects give rise to a change in the band-edge structure and raise the ground-state energy of the free carrier, which is reflected in increases in the optical band gap and electrical resistivity. It is then of great interest to explore how carrier transport properties are modified by reduced dimensionality due to the quantum confinement from the viewpoints of basic physics of a disordered system. Another interesting aspect of multilayered structures is the possibility of investigating the effects of interface on carrier transport with extended detection sensitivity, which matches the requirement from the view of device physics.

In this work we investigate the in-plane carrier transport in hydrogenated amorphous silicon (a-Si:H)/silicon carbide (a-SiC:H) multilayered structures of various sublayer thicknesses. The transient grating method is employed for this purpose, which enables us to separately determine the diffusion coefficient $D$ and the lifetime $\tau$ of photoexcited carriers confined within the a-Si:H well layers. We find that the diffusion coefficient exhibits a monotonous decrease with decreasing a-Si:H well layer thickness $L_w$, while the carrier lifetime increases to keep the $D\tau$ product constant for $L_w \geq 100$ Å and then shows a drastic increase for $L_w \leq 50$ Å. These phenomena are interpreted as arising from the combined effect of carrier interaction with shallow traps at the a-Si:H/a-SiC:H interfaces and weakened carrier coupling with deep states in a-Si:H well layer due to the quantum-size effect.

The multilayered structures were prepared on glass substrates by rf plasma chemical vapor deposition using a 1:9 SiH$_4$/H$_2$ gas mixture for the a-Si:H layers and a 1:13:126 SiH$_4$/CH$_4$/H$_2$ gas mixture for the a-SiC:H layers. Each layer was formed in separate chambers with interruption on the plasma. The thicknesses of the sublayers were determined by the deposition time and the deposition rates for the thick films. The a-Si:H well layer thickness was varied from 20 to 1000 Å while keeping the total well layer thickness at 3000 Å, and the a-SiC:H barrier layer thickness was fixed at 100 Å to avoid interlayer carrier tunneling. The optical band gaps were 1.75 and 2.80 eV for a-Si:H and a-SiC:H, respectively, which were determined from the optical absorption spectra of identical thick films following the Tauc plot.

In the transient grating method, two excitation light pulses of wavelength $\lambda_p$, separated by an angle $2\theta$, are focused onto the multilayer sample so that they both spatially and temporally coincide as shown in Fig. 1. The direct absorption of excitation pulses produces a spatially modulated carrier density with a periodicity $\Lambda = \lambda_p / 2 \sin \theta$. When the photon energy of excitation light is selected to be an appropriate value which situates between both band-gap energies of sublayers, photocarrier generation predominantly takes place within the well layers. Following the generation, the free-carrier grating decays by in-plane diffusion and recombination in the well layers. The grating decay is monitored by observing the first-order diffracted light from a probe light of a wavelength $\lambda_E$. The decay time constant $(T/2)$ of diffracted light is related to the carrier diffusion coefficient $D$ and lifetime $\tau$ by an equation $1/T = 1/\tau + 4\pi^2D / \Lambda^2$. Therefore, the measurement of the time constant $T$ at various grating pitches (i.e., $\theta$) allows us to separately determine the diffusion coefficient $D$ and lifetime $\tau$.

FIG. 1. Schematic diagram of the transient grating method. In a multilayer sample, the transient grating is selectively formed within the well layers.
The second harmonics ($\lambda_2 = 532$ nm) from a Q-switch yttrium aluminum garnet (Q-SW YAG) laser was used as the excitation light pulse, and the pulse width (FWHM) and excitation power were approximately 8 ns and 1 MW/cm$^2$, respectively. The photon energy of the excitation light is $2.33$ eV, at which the absorption coefficient of a-Si:C:H of $2.80$ eV band gap is more than two orders of magnitude smaller than that of a-Si:H of $1.75$ eV band gap so that photocarrier generation is entirely negligible in the a-Si:H barrier layers. The light from a He-Ne laser ($\lambda_p = 632.8$ nm) with a duration of 8 ns and an intensity of 1 W/cm$^2$ was directed onto the sample to probe the transient grating. The diffracted probe light was observed by a photomultiplier and a transient digitizer.

The diffusion coefficient $D$ and the lifetime $\tau$ are determined from the linear relation between the measured value of $1/T$ and $4\pi^2/k^2$. The results obtained for the multilayered structures are summarized in Fig. 2(a), as a function of the well layer thickness $L_w$. Corresponding quantities of an unlayered thick (bulk) a-Si:H film are also shown for comparison. It is found that the lifetime in the multilayered structure of $L_w = 1000$ Å is slightly smaller than that in the bulk material, while the diffusion coefficient is almost identical in each specimen. In multilayered structures, the interface is considered to be highly disordered due to the morphological and compositional fluctuation so that localized states of large density would exist at this region. The observation, however, indicates that the a-Si:H/a-Si:C:H interface involves only a small number of defects which play a significant role in determining carrier transport as deep-trapping centers.

When decreasing the thickness of the well layer from 1000 to 20 Å, the diffusion coefficient gradually decreases from $1.2 \times 10^{-2}$ to $2.6 \times 10^{-5}$ cm$^2$/s, while the lifetime remarkably increases from 0.7 to 40 µs. Figure 2(b) shows the variation of the diffusion length $(D\tau)^{1/2}$, which is almost unchanged and kept at $0.8 \mu$m in the region from 100 to 1000 Å. With decreasing $L_w$ below 50 Å, it increases up to 3.2 μm due to the increase in the lifetime. In the region where $(D\tau)^{1/2}$ is almost constant, it is likely that shallow-trapping effects mainly dominate the carrier transport. Suppose that such shallow traps originate from disordering at the interfaces and locate within a narrow region of the interface. Then, according to the trap-controlled transport model which includes carrier interaction with the shallow states, both the transport parameters $D$ and $\tau$ are expected to follow the relations

$$D \approx \frac{D_0}{1 + \beta N_f/L_w},$$

$$\tau \approx \tau_0 (1 + \beta N_f/L_w),$$

where $N_f$ (cm$^{-2}$) denotes the density of shallow traps at the interface and $\beta$ is a coefficient which is inversely proportional to the effective density of states $N_{eff} (-10^{20}$ cm$^{-3}$)$^6$ in the extended band. $D_0$ and $\tau_0$ are the relevant quantities inherent in the well layer. The above equations hold well, as long as carrier transport in each well layer is isolated from that in neighboring sublayers and the well layer thickness is considerably smaller than the carrier diffusion length. It is suggested that the effect of shallow traps at the interface is apparently equivalent to that of shallow traps uniformly distributed in the well layer with the density $N_f/L_w$. As indicated by the solid lines in Fig. 2, Eqs. (1) and (2) give reasonable fits to experimental data by using a parameter $\beta N_f = 10^{10}$ cm, except for the lifetime data in the thin well layer region ($L_w < 50$ Å). Since the $\beta N_{eff}$ product should be larger than unity, the density $N_f$ is estimated to be $10^{14}$ cm$^{-2}$ at maximum.

The classical shallow-trap model can satisfactorily explain layer-thickness dependences of the carrier diffusion coefficient and lifetime in the moderately thick well layer region. Another concern of our discussion is then placed on the implication of the increase in the carrier lifetime observed in the thickness range $L_w < 50$ Å. The recent extensive work on the optical and electrical properties of layered amorphous semiconductors has led to a conclusion that quantum-size effects become important in such a thin layer region.

Quantum confinement in a sufficiently deep square potential well raises the ground-state energy of free carrier by a factor proportional to $1/L_w^2$, if the coherence of the wave function is larger than $L_w$. This effect is reflected in an increase in the optical band gap with a linear dependence on $1/L_w^2$, which is confirmed for the present multilayer system as shown in Fig. 3(b). Besides such behavior of the optical band gap, Tiedje et al. observed an increase in the in-plane
resistivity, and found that the increase is also well interpreted on the basis of the quantum well model. This finding suggests that the mobility edge shifts higher due to the quantum confinement, and is not largely influenced by the localization effect induced by reduced dimensionality. The direct measurement of the diffusion coefficient indicates that the localization effect is actually negligible in the thickness region $L_w < 50 \text{ Å}$, where the free carrier becomes two dimensional due to quantum confinement.

The shift of the mobility edge toward the higher energy brings about an increase in the energy separation between the transport state and the deep state involved in the carrier-capture process. If the multiphonon emission process dominates the carrier capture into the deep states, the capture probability, and thereby, the lifetime $\tau_0$, should be determined by the multiphonon rate which exponentially depends on the energy released in the capture process. Therefore, we expect that the lifetime $\tau_0$ depends exponentially on the extent of the band-edge shift, that is, $1/L_w$. To confirm this, we plot the logarithm of the lifetime $\tau_0$ as a function of $1/L_w^2$ in Fig. 3(a). The excellent linearity between $\ln(\tau_0)$ and $1/L_w^2$ found in this figure indicates the plausibility of the model described above.

In conclusion, we have performed a direct measurement of carrier transport properties in the $\alpha$-Si:H/$\alpha$-SiC:H multilayered structure. Localized states at the $\alpha$-Si:H/$\alpha$-SiC:H interface play an important role in determining parallel carrier transport mainly as the shallow traps. The effect results in, when decreasing the well layer thickness, a decrease in the diffusion coefficient and an increase in the lifetime, while keeping their product unchanged. When carriers are confined within narrower well layers of thickness below $50 \text{ Å}$, the reduced dimensionality due to quantum confinement gives rise to a weakened carrier coupling with deep-trapping centers so that the carrier lifetime drastically increases by about one order of magnitude as compared with that of three dimensions. At such a thin thickness range, where carriers become two dimensional, the diffusion coefficient remains at a finite value contrary to the theory of localization in the two-dimensional disordered system.

![Figure 3](image)

**FIG. 3.** (a) Carrier lifetime $\tau_0$ and (b) optical band gap as a function of the factor of quantum confinement $1/L_w$. The lifetime $\tau_0$ is derived from measured lifetime according to the equation inserted in the figure. Solid lines are theoretical plots calculated on the basis of the quantum well model.