Unified Set of Models for Minority Carrier Transport Parameters in Heavily Doped Monosilicon and Polysilicon

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The importance of heavily doped mono- and polysilicon in advanced devices such as polysilicon emitter contacts and the increasing use of simulation in development and manufacturing has created a need for accurate transport parameter models for minority carriers. Numerous transport parameter models for heavily doped silicon have been proposed, but disagreement still exists over which are correct, and models for minority carrier transport parameters in heavily doped polysilicon are virtually nonexistent. In this paper we present a complete set of models for minority carrier transport parameters (mobility, lifetime, and bandgap) in heavily doped n-type mono and polysilicon. The models are analytic functions of doping and temperature. The models for polysilicon are also functions of grain microstructure. They predict behavior which agrees with the most recent available data and models, and they are easily implemented in device simulators. Self-consistency implies that when used as a set in the solution of the transport and current equations, the models predict correct results. Two authors [1, 2] have published complete, self-consistent sets of models for steady state minority carrier transport parameters in heavily doped silicon but models for the transport parameters differ between the two. Recent work [3, 4] has supported the models published by [1] for bandgap narrowing and mobility, respectively, thus we use the empirical models in [1] as a basis for our work.

Our monosilicon work focuses on effective bandgap narrowing, $\Delta E_{g,eff}$, which is critical for modeling changes in intrinsic carrier concentration due to heavy doping. In contrast to theoretical models, i.e.[4, 2, 5], the validity of empirical models based on measurements of $\Delta E_{g,eff}$, [1, 3], is limited to the range of doping in devices measured, approximately $5 * 10^{18} < N_d < 10^{20} cm^{-3}$. A consistent and important difference between the theoretical models and the empirical models is that the empirical models predict that $\Delta E_{g,eff}$ increases monotonically with doping, while the theoretical models show that the relationship is non-monotonic at higher doping. This nonmonotonicity at high doping levels is a result of bandgap widening effects from degeneracy. We use a slightly modified form of the model from [2]. It includes physical considerations of degeneracy as well as band structure changes and predicts the correct non-monotonic behavior at high doping levels. Our $\Delta E_{g,eff}$ model is shown in Figure 1 along with empirical $\Delta E_{g,eff}$ models proposed by [1] and [3]. The magnitude of our model matches well to the empirical models.

The models we propose for lifetime and mobility are given in Table 1. The mobility model is based on models of [1] and [6]. The lifetime model includes Auger and Shockley-Hall-Read recombination. In heavily doped silicon, Auger recombination dominates in the determination of the lifetime. Dziewior et.al. [7] showed that the minority carrier lifetime has a negligible dependence on temperature for the range $77K < T < 400K$.

In polysilicon, carrier mobilities and lifetimes depend not only on doping concentration and temperature but also on grain microstructure. It is widely viewed that transport parameters inside grains are the same as those in monosilicon, but that behavior of carrier mobilities and lifetimes at the grain boundaries are quite different from those in monosilicon. The polysilicon mobility and lifetime values are combinations of the values within the grains and at the grain boundaries.

In our polysilicon mobility model we assume that minority carrier transport behaves similarly to majority carrier transport and we adopt the form proposed in [8] for modeling majority carrier mobility in heavily n-type polysilicon. We model transport inside grains as in monosilicon and transport in grain boundaries as in [8]. Electron mobility in n-type polysilicon was studied in [8]. Since hole mobility in heavily-doped n-type silicon is about half of the electron mobility, we assume this relationship holds in polysilicon and include this factor in our grain boundary mobility model for holes. The expression for effective mobility in polysilicon, μ_{poly}, combines grain and grain boundary mobilities. Our model requires parameters l_g, average grain size, and N_g, average number of grains seen by a carrier. The number of grain boundaries, N_{gb} is related to N_g by $N_{gb} = N_g - 1$. The model for the effective mobility is given in Table 1. In the equation, W_{poly} is the width of the poly layer, l_g and l_{gb} are the grain and grain-boundary length, respectively, and μ_g and μ_{gb} are the mobilities in the grains and in the grain boundaries, respectively.

Significant recombination takes place at the grain boundaries in polysilicon. For smaller grains there is a larger proportion of grain boundaries and correspondingly greater recombination. Thus, lifetime, τ_{poly} is related to grain size. A relation which fits the data well for effective lifetime in the grain boundaries is $\tau_{gb}(sec) = 5 * 10^{-6} * l_g$, where l_g is the grain size in cm [9]. Our model for lifetime in polysilicon is given in Table 1. We model $\Delta E_{g,eff}$ in polysilicon the same as $\Delta E_{g,eff}$ in monosilicon, which is a function of doping concentration in the grains and temperature.

Our models' predictions of minority carrier diffusion length in polysilicon, $L_{poly} = \sqrt{D_{poly}\tau_{poly}}$, as functions of temperature and number of grains are shown in Figure 2. Only one work, [10], has reported measured L_{poly} in polysilicon doped to $10^{20}cm^{-3}$. They [10] report room temperature values of L_{poly} of $41nm$ and $50nm$. These results match well to our model for $Ngrains \sim 3$. Note also that the model approaches values for monosilicon at $Ngrains = 1$, which makes the models useful for polysilicon applications where anneal conditions may result in recrystallized monosilicon.

In summary, we have presented a complete set of transport parameter models for minority carriers in heavily doped mono and polysilicon. The models match well with the most recent available data and models for minority carrier transport. They include dependencies on doping level and grain size and are easily implemented in device simulators.

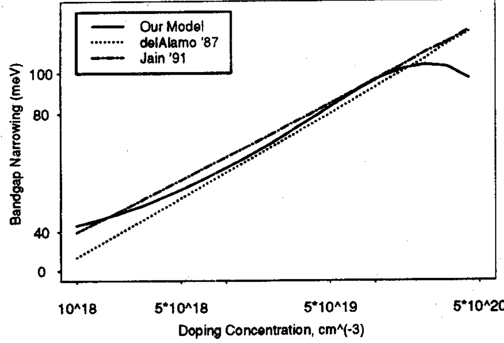

Figure 1: Bandgap Narrowing vs. Doping Concentration for Different Models.

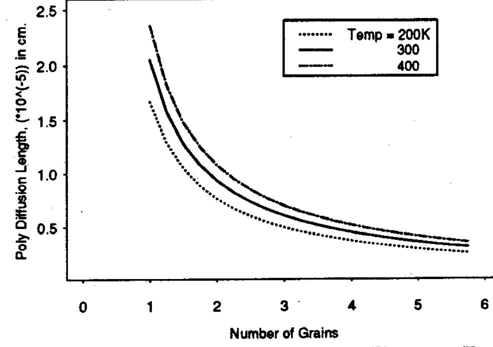

Figure 2: Diffusion Length in Polysilicon as Function of Number of Grains and Temperature.

Material	Parameter Name	Model	Source
MONO SILICON	Bandgap Narrowing	$\Delta E_{g,eff} = \Delta E_{gN} - \Delta E_{gD}$. $\Delta E_{gN} = An^{0.36}$ $\Delta E_{gD} = kTR_N \left[64 + 0.05524 R_N (64 + R_N^{0.5})\right]^{-0.25}$ $A = 0.8 * 10^{-8}$, $R_N = \frac{n}{N_C}$, n is ionized carrier concentration; N_C is density of states.	Form from [2]; Modified Values to agree with [1]
	Intrinsic Bandgap	$E_{go} = 1.1785 - 9.025 * 10^{-5}T - 3.05 * 10^{-7}T^2$, $(150K < T < 300K)$ $E_{go} = 1.206 - 2.73 * 10^{-4}T$, $(250K < T < 450K)$	[11]
	Mobility	$\mu_p = \mu_{min} + \frac{\mu_{max} - \mu_{min}}{1+\left(\frac{N_d}{2.2*10^{17}}\right)} \frac{cm^2}{V \cdot s}$. $\mu_{min} = 129$, $\mu_{max} = 461$.	[1] and [6]
	Lifetime	$\frac{1}{\tau_p} = \frac{1}{\tau_{srh}} + \frac{1}{\tau_{Aug}}$ $\tau_{srh} = \frac{\tau_o}{1+\frac{N_d}{N_{ref}}}$; $\tau_{Aug} = \frac{1}{C_A N_d^2}$; $C_A = 1.8 * 10^{-31} cm^6/s$, $\tau_o = 10\mu s$, $N_{ref} = 10^{17}/cm^3$.	[1] and [6]
POLY-SILICON	Bandgap Narrowing	$\Delta E_{g,eff}$ model as in monosilicon. n is doping level inside grains.	
	Mobility	$\mu_{poly} = W_{poly} \left[\frac{N_g l_g}{\mu_g} + \frac{(N_g - 1) l_{gb}}{\mu_{gb}}\right]^{-1}$ $\sigma_{gb}(T) = \sigma_0 exp\left[\frac{-E_H}{kT}\right] + \sigma_1 exp\left[\frac{-E_L}{kT}\right]$ $\mu_{gb} = \frac{\sigma_{gb}}{qn}$. μ_g is mobility in monosilicon. $E_H > E_L$ and $\sigma_0 > \sigma_1$.	
	Lifetime	$\frac{1}{\tau_{poly}} = \frac{1}{\tau_g} + \frac{1}{\tau_{gb}}$ $\tau_{gb}(sec) = 5 * 10^{-6} * l_g$, τ_g is lifetime in monosilicon.	

Table 1: Minority Carrier Transport Models for Heavily-doped n-type Monosilicon and Polysilicon

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