

Dynamics of p^+ polysilicon gate depletion due to the formation of boron compounds in $TiSi_2$

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Abstract

In dual workfunction gate technologies it can be observed, that p^+ poly gates of pMOSFETs tend to lose boron doping. This work presents a model for the transport of Si and B in the $TiSi_2$ /polysilicon bilayer system that can explain the saturation of the B dose loss.

1 Introduction

Many CMOS applications are driven by low power and high performance issues. Both demands can be met by the dual workfunction gate technology (p^+ poly gates for pMOSFETs and n^+ poly gates for nMOSFETs). It is observed, that p^+ poly gates of pMOSFETs tend to lose boron doping [1]. Depletion of gate degrades the performance of pMOSFETs. On the other hand for metallization titanium disilicide $TiSi_2$ was shown to have low sheet resistance and low contact resistance on p and n type silicon. The focus of this work is to provide insight to the boron transport in the $TiSi_2$ /polysilicon bilayer system.

2 Experimental

Fig. 1 shows boron profiles from secondary ion mass spectrometry (SIMS) after anneals at $900^\circ C$ for 1, 10 and 60 minutes. Fig. 2 shows corresponding boron doses in polysilicon (from Fig. 1, thickness of the polysilicon layer: $0.170\mu m$) as a function of the anneal time. A pronounced dose loss is observed after 10min. For larger times the boron dose saturates.

3 Theory

The boron kinetics in $TiSi_2$ is dominated by the formation of titanium diborides TiB_2 [2], i.e. by



The corresponding law of mass action is

$$C_{TiSi_2}(C_B^t)^2 = K_1 C_{TiB_2}(C_I^t)^2, \quad (2)$$

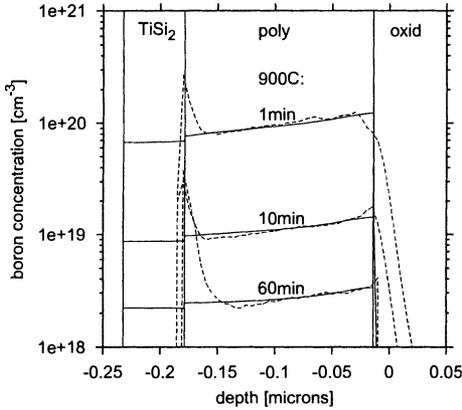


Figure 1: Boron distributions from SIMS (dashed lines) and from simulation (solid lines) after annealing at 900 °C for 1, 10 and 60 minutes.

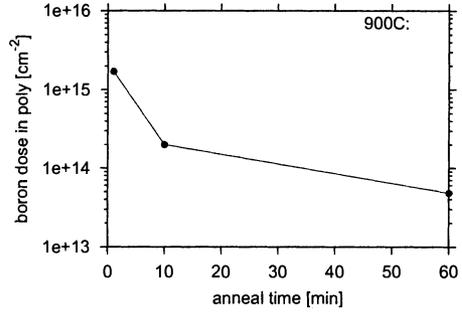


Figure 2: Boron dose in polysilicon (from Fig. 1) as a function of the anneal time at 900 °C.

where C_{TiSi_2} , C_B^t , C_{TiB_2} and C_I^t are the volume concentrations of $TiSi_2$, mobile B, TiB_2 and of mobile silicon atoms respectively. The superscript 't' indicates mobile species in the $TiSi_2$ matrix, K_1 is a mass action constant. The concentration of molecules in the host material C_{TiSi_2} is assumed to be constant ($K = C_{TiSi_2}/K_1$), leading to

$$C_{TiB_2} = K(C_B^t)^2/(C_I^t)^2. \quad (3)$$

The reaction (1) is assumed to be in equilibrium on the time scale of dopant diffusion and other reactions. Thus the concentrations C_B^t , C_{TiB_2} and C_I^t cannot change independently over time, but satisfy

$$\frac{d}{dt} C_{TiB_2} = \frac{d}{dt} K + 2 \frac{d}{dt} C_B^t - 2 \frac{d}{dt} C_I^t. \quad (4)$$

The first term shows up because K implicitly depends on time by the temperature dependence of the mass action constant. It can be neglected when only constant temperature processing is taken into account. As this applies to the present investigation the first term will be neglected further on. Boron and silicon can diffuse through the $TiSi_2$ material. The according continuity equations are

$$\frac{d}{dt} C_B^t = \nabla \cdot j_B^t - 2 \frac{d}{dt} C_{TiB_2} \quad (5)$$

$$\frac{d}{dt} C_I^t = \nabla \cdot j_I^t + 2 \frac{d}{dt} C_{TiB_2} - R_I^t. \quad (6)$$

The current densities are given by simple diffusion terms, i.e. $j_B^t = D_B^t \nabla C_B^t$, $j_I^t = D_I^t \nabla C_I^t$ where D_B^t , D_I^t are the diffusivities of boron and silicon in $TiSi_2$.

In analogy to point defect models in silicon substrate mobile silicon recombine to an equilibrium concentration $C_I^{eq,t}$. The relaxation rate is assumed to be $R_I^t =$

$(C_I^t - C_I^{eq,t})/\tau_I^t$ with relaxation time τ_I^t . Combining eq. (4)–(6) we obtain

$$\alpha_{11} \frac{d}{dt} C_B^t - \alpha_{12} \frac{d}{dt} C_I^t = \nabla \cdot j_B^t \quad (7)$$

$$\alpha_{21} \frac{d}{dt} C_I^t - \alpha_{22} \frac{d}{dt} C_B^t = \nabla \cdot j_I^t - R_I^t \quad (8)$$

with

$$\begin{aligned} \alpha_{11} &= (1 + 4C_{TiB_2}/C_B^t) & \alpha_{12} &= 4C_{TiB_2}/C_I^t \\ \alpha_{21} &= (1 + 4C_{TiB_2}/C_I^t) & \alpha_{22} &= 4C_{TiB_2}/C_B^t. \end{aligned}$$

The boron transport in polysilicon is dominated by a two stream diffusion [3, 4]. Boron atoms diffuse in the grain interior C_B^{gi} and in grain boundaries C_B^{gb} . Diffusivity in grain boundaries is much faster than in grains. Dopants segregate between grain interior and grain boundaries with a rate G_s

$$\frac{d}{dt} C_B^{gi} = \nabla \cdot j_B^{gi} - G_s \quad (9)$$

$$\frac{d}{dt} C_B^{gb} = \nabla \cdot j_B^{gb} + G_s \quad (10)$$

$$G_s = t(C_{B,max}^{gb} - C_B^{gb})C_B^{gi} - e(C_{B,max}^{gi} - C_B^{gi})C_B^{gb}. \quad (11)$$

The trapping rate (kinetic coefficient t) of boron from grain interior to grain boundaries is proportional to free states on grain boundaries ($C_{B,max}^{gb} - C_B^{gb}$) and to filled states in grain interior C_B^{gi} . The emission rate (kinetic coefficient e) in the opposite direction is proportional to free states on grain interior ($C_{B,max}^{gi} - C_B^{gi}$) and to filled states in grain boundaries C_B^{gb} . $C_{B,max}^{gb}$ is the maximum boron concentration in grain boundaries and depends on the local grain size. $C_{B,max}^{gi}$ is the maximum boron concentration in grain interior and is given by the solid solubility.

Usually polysilicon diffusion models do not include point defect kinetics. However the grain boundaries are known to absorb interstitials very effectively [5]. From the reaction (1) it can be expected that much mobile silicon is generated during the formation of TiB_2 . These silicon atoms enter the polysilicon as interstitials and recombine at grain boundaries. To account for this the polysilicon diffusion model was extended by a simple continuity equation for interstitials

$$\frac{d}{dt} C_I^p = \nabla \cdot j_I^p - R_I^p. \quad (12)$$

C_I^p is the concentration of interstitials in polysilicon. The recombination rate in polysilicon is $R_I^p = (C_I^p - C_I^{eq,p})/\tau_I^p$.

4 Results

The above equations have been implemented in PROMIS-NT [6]. Although some model parameters in $TiSi_2$ and polysilicon are not well known the proposed model provides insight into the underlying physical mechanisms:

At the beginning of the process B diffuses into $TiSi_2$ and starts reaction (1). The generated mobile silicon recombines in $TiSi_2$ (rate R_I^t in eq. (8)), outdiffuses into the polysilicon and recombines here too (rate R_I^p in eq. (12), Fig. 3). When the silicon concentration in $TiSi_2$ approaches its equilibrium value, Fig. 4, reaction (1) stops. Consequently the outdiffusion of B into $TiSi_2$ also stops. In effect the presented model for the $TiSi_2$ /polysilicon bilayer system can explain the saturation of the B dose loss, Fig. 2.

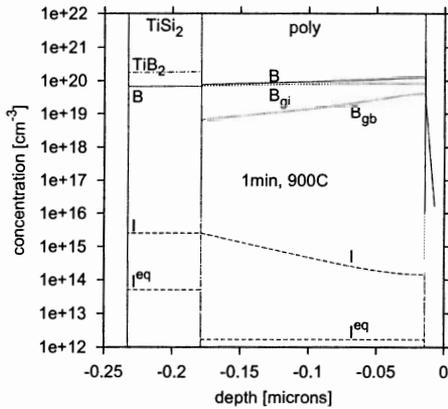


Figure 3: Distribution of solved model species boron (labeled as B in TiSi_2 and as B_{gb} , B_{gi} , B in poly), mobile silicon in TiSi_2 and silicon interstitials in poly (both labeled as I) after a 1 minute anneal at 900°C . TiB_2 results from eq. (3).

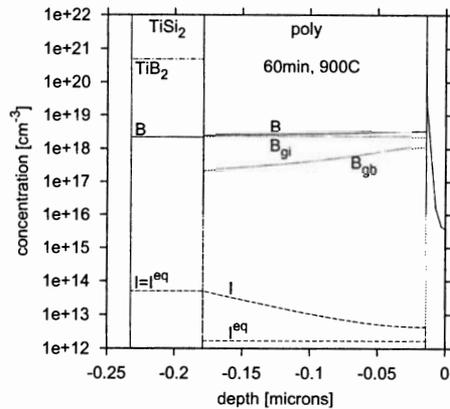


Figure 4: Distribution of model species after a 60 minute anneal at 900°C .

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