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Modeling of gettering of precipitated impurities from Si for carrier lifetime improvement in solar cell applications

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Physical and numerical modeling of impurity gettering from multicrystalline Si for solar cell production has been carried out using Fe as a model impurity. Calculated change of nonradiative recombination coefficient of minority carriers in the course of gettering is used as a tool for evaluating the gettering efficiency. A derivation of the capture cross section of impurity precipitates, as compared to single atom recombination centers, is presented. Low efficiency of the conventional application of the gettering process is explained by the modeling results. The variable temperature gettering process is modeled and predicted to provide high gettering efficiency and short needed gettering times. © *1999 American Institute of Physics.* [S0021-8979(99)00717-3]

I. INTRODUCTION

A large minority carrier recombination lifetime or long diffusion length in Si is essential for achieving high efficiencies of silicon-based solar cells. Therefore, it is desirable to minimize the concentration of recombination centers in Si wafers used for solar cell applications. Such recombination centers include the structural defects, e.g., dislocations, grain boundaries, twins, etc., as well as metallic impurity atoms dissolved in the Si matrix and their precipitates. Gettering is known to be an effective way of minimizing the concentration of impurities in Si. Unlike the case of integrated circuits for which devices are situated in a thin layer at the wafer surface, solar cells use the whole bulk of the wafer as the active device region and hence recombination center concentrations must be minimized in the entire wafer bulk. This is the reason that *intrinsic gettering*,[1] which is the standard technique used in integrated circuit (IC) fabrications and consists of removing metallic contaminants from the Si wafer surface region to the wafer bulk, is not suitable for solar cells.

Only extrinsic gettering methods can be effective for removing metallic impurities from the whole bulk of a Si wafer. Such methods include gettering by a liquid aluminum layer (LAL), by P in-diffusion, and by wafer surface damages. It has been shown that LAL gettering can significantly increase minority carrier diffusion lengths and hence also lifetimes in Czochralski Si,[2] but the effectiveness of the method is limited for commercial or low cost *multicrystalline* (MC) Si containing metallic impurities in high concentrations.[3,4] In MC Si, besides dissolved impurities, there is also an abundance of structural defects which serve as preferential sites for metal silicide precipitates to form. For successful gettering, it is necessary to completely dissolve such precipitates since they serve as sources that slowly release metal atoms into the Si matrix during the gettering process. In a preliminary modeling study, we have found that, because the process of silicide precipitate dissolution is extremely slow, it takes as long as 60 h or more at 700 °C to *complete* the gettering process of Fe, which has been introduced to the solubility limit at the 900 °C and subsequently a fairly high density of precipitates has been formed at 700 °C.[4] Here *completion* of the gettering process means to completely dissolve all precipitates and subsequently the dissolved impurity atoms reached the steady state distribution in the gettered and gettering regions. Increasing the gettering temperature can accelerate the precipitate dissolution process and increase the diffusion coefficient of dissolved metal atoms. However, at a higher gettering temperature, the metal solubility is much larger and the needed precipitate dissolution completion time can still be fairly long. Thus, it is possible to result in worsened carrier lifetimes for cases for which the gettering times are shorter than the needed completion time of the gettering process. This provides a possible explanation of the experimentally observed degradation of low cost Si solar cell performance after a short time gettering at 950 °C.[5,6] Moreover, also because of the increased metal solubilities at the higher gettering temperatures, the gettering driving force, which is the metal segregation coefficient between LAL and Si, is smaller, resulting in the fact that the ultimately attainable metal concentration is larger than that attainable at a lower gettering temperature. Thus, the choice of the gettering temperature is a compromise between diffusion coefficient and precipitate dissolution on the one hand and segregation coefficient on the other hand. Modeling of the process of gettering presented in this article confirms the above assessment.

In this article we will concentrate on the modeling of the LAL method for the gettering of metallic impurities in MC Si wafers used for commercial solar cell fabrications. The modeled aspects include the impurity atom diffusion and segregation processes, and the precipitate dissolution pro-

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[c)] Electronic mail: ttan@acpub.duke.edu cess. Furthermore, a derivation of the carrier capture cross section of impurity precipitates, as compared to single atom recombination centers, is presented. In order to improve the gettering efficiency and to shorten the needed gettering times, we propose a variable temperature gettering scheme. To estimate the effectiveness of gettering, the recombination coefficient of minority carriers diffusing through silicon wafer from one surface to the other is used. It takes into account the recombination on the centers formed by both dissolved and precipitated impurity.

II. GETTERING MECHANISMS AND FUNDAMENTAL EQUATIONS

An Al layer on the Si wafer surface provides gettering effect because of chemical segregation. The solubility of most metals in Al is very high, reaching 1 at. % in solid Al. Above the eutectic temperature of 577 °C, wherein a liquid Al–Si alloy forms, the solubility of metals can typically exceed 10 at. %, or $5\times10^{21}\,\mathrm{cm}^{-3}$. Since the solubility limit of metals in Si does not exceed $\sim10^{17}\,\mathrm{cm}^{-3}$, their segregation coefficient between the Al–Si liquid and Si is higher than 10^4, reaching 10^{10} for many metals. This provides a tremendous driving force for metal atoms to segregate into the Al–Si liquid layer. This gettering method should be highly effective for interstitial metal species because of their large segregation coefficients and diffusivities in Si. Al itself has a relatively low diffusivity in Si compared to most other metals. Solar cell efficiencies can be improved by the use of Al for a variety of reasons, with gettering being an important contributor.[2] Because of the involvement of the segregation processes, which occur simultaneously with the impurity diffusion, the gettering process is in general described by the diffusion-segregation equation[7]

$$\frac{\partial C}{\partial t}=\frac{\partial}{\partial x}\left[D\left(\frac{\partial C}{\partial x}-\frac{C}{m}\,\frac{\partial m}{\partial x}\right)\right], \tag{1}$$

where m is the segregation coefficient of the gettered impurity species. The value of m equals 1 in Si, and in the Al–Si melt layer equals the ratio of the metal solubilities in the Al–Si layer and in Si. For segregation occurring at an abrupt junction, e.g., at the interface of LAL and Si, one can also use the empirical computational flux criterion[8]

$$j_s=h\left(C_1-\frac{C_2}{m_2}\right), \tag{2}$$

where j_s is the flux density at the Si and Al–Si liquid interface, C_1 is the impurity concentration at the last computational grid point at the Si side of the interface, C_2 is the impurity concentration at the first computational grid point at the Al–Si liquid side of the interface, m_2 is the impurity segregation coefficient (for the LAL gettering case it is the impurity segregation coefficient in the Al–Si melt relative to Si), and h is the *mass transport* coefficient. It has been recently shown that[9] $h=D^{\mathrm{eff}}/\lambda$, where D^{eff} is an effective diffusivity through the transition layer between Si and LAL, and λ is the thickness of the transition layer. Except for an extremely short period immediately after the onset of the gettering process, the impurity gettering rate is limited by its diffusion in Si bulk to the LAL–Si interface, rather than the chemical reaction of impurity transition from Si into Al. This means we may consider the gettering process as one for which the impurity concentration reached a quasisteady state in the LAS–Si system, which allows us to assume that $j_s \ll hC_1$ and $j_s \ll hC_2/\mathrm{m}$ hold. Hence, for our present problem, Eq. (2) reduces to

$$C_{\mathrm{LAL}}\approx mC_{\mathrm{Si}}, \tag{3}$$

which is a boundary condition independent of the computational grid.

To treat the problem of LAL gettering of precipitated impurity, a set of four equations has been developed

$$\frac{\partial C}{\partial t}=D\,\frac{\partial^2 C}{\partial x^2}+4\pi r\rho D(C^*-C), \tag{4}$$

$$C^*=C^{\mathrm{eq}}\exp\left(\frac{2\Omega\gamma}{rk_BT}\right), \tag{5}$$

$$\frac{dr}{dt}=-\frac{\Omega D}{r}(C^*-C), \tag{6}$$

$$\frac{dC_{\mathrm{get}}}{dt}=-\frac{D}{d_{\mathrm{get}}}\left(\frac{\partial C}{\partial x}\right)_{x=0} \tag{7}$$

for which the precipitates are assumed to be spherical in shape, for simplicity. In Eqs. (4)–(7), C is the impurity (metal) atom concentration in the Si matrix, C^* is the impurity dynamic equilibrium concentration at the interface of Si and the precipitate with radius r, C^{eq} is the thermal equilibrium concentration of the impurity, ρ is the precipitate density, Ω is the volume of precipitate per one impurity atom, γ is the precipitate-matrix interfacial energy density, k_B is Boltzmann's constant, and d_{get} is the thickness of the LAL gettering layer. It is noted that Eqs. (4)–(7) apply to the precipitate growth as well as dissolution processes. It was assumed that the impurity diffuses sufficiently fast in the liquid Al layer, so that its concentration can be considered uniform in that layer.

III. CALCULATION OF RECOMBINATION RATE

In the process of photocurrent/voltage generation in Si solar cell by photons, electron-hole pairs are created and separated to the two wafer surfaces by a junction electric field and by carrier diffusion. The electron-hole pairs are generated mostly near the front surface of the wafer, and to a lesser extent in the bulk. However, for the purpose of estimating the carrier recombination rate in the Si bulk, we will consider only the carriers near the back surface because of the longer distance they have to travel as minority carriers to reach the *p*-*n* junction. To increase the cell efficiency, the number of minority carriers reaching the *p*-*n* junction should be maximized, which can be achieved by providing a wafer back surface field and by decreasing the minority carrier recombination rate in the bulk of the wafer via impurity gettering. For the purpose of evaluating the effectiveness of the gettering process, we consider only the process of electrons diffusing as minority carriers through the *p*-type Si wafer bulk containing recombination centers. Within a local diffusion domain, the excess electrons are also diffusing to each of these centers to recombine with holes. With all the excess electrons assumed to be generated at the wafer back surface, i.e., at $x=0$, the average excess concentration of electrons at depth x may be represented by

$$\delta\overline{n}(x)=\delta\overline{n}(0)\exp\left(-\int_0^x \frac{\alpha_{\mathrm{rec}}(x)}{v_{\mathrm{dif}}}\,dx\right), \tag{8}$$

where v_{dif} is the average speed of electron diffusion from the back to the front of the wafer, and α_{rec} is the recombination constant expressed as

$$\alpha_{\mathrm{rec}}=v_{\mathrm{th}}\sum_i C_i\sigma_i, \tag{9}$$

where v_{th} is thermal velocity of minority carriers, C_i is concentration of the ith-type of recombination centers, and σ_i is their carrier capture cross section. For a given impurity, possible types of recombination centers are dissolved individual impurity atoms and impurity-containing precipitates. In this work, we assume that all impurity precipitates at a certain depth x have the same size, and hence the same capture cross section. Otherwise, a summation (or integration) with respect to the size of precipitates is needed in Eq. (9). It should be noted that the additive contribution of an impurity to the recombination constant becomes multiplicative when the percentage of nonrecombined minority carriers is calculated, according to Eq. (8). Thus, the presence of an impurity at a certain concentration is equally crucial in high and low quality material, regardless of the concentration of other impurities and extended defects.

We propose to characterize the contribution of an impurity to the recombination of minority carriers on their way from the vicinity of the back surface to the front surface by the *relative integrated recombination constant*

$$\alpha^*=\frac{\int_0^d[C_{\mathrm{sol}}(x)\sigma_{\mathrm{sol}}+C_{\mathrm{ppt}}(x)\sigma_{\mathrm{ppt}}]dx}{d_{\mathrm{Si}}(C_{\mathrm{sol}}^o\sigma_{\mathrm{sol}}+C_{\mathrm{ppt}}^o\sigma_{\mathrm{ppt}})}, \tag{10}$$

where d_{Si} is the thickness of the wafer, the subscript sol stands for dissolved impurity atoms in solution and ppt for precipitates, and the superscript 0 stands for an appropriate reference value prior to gettering, which is assumed to be uniformly distributed in the wafer. Thus, in a situation of nonuniform time-dependent distribution of recombination centers of various kinds, α^* is a very demonstrative and inclusive measure of the minority carrier recombination rate.

In order to calculate α^*, it is necessary to evaluate $\sigma_{\mathrm{ppt}}/\sigma_{\mathrm{sol}}$ as a function of the precipitate size. For this purpose, we need to first decide whether the carrier recombination process at a center is limited by a potential barrier at the center or by diffusion of the minority carries to the center. It is known that the electron-hole recombination reaction time at a center possessing a deep level is on the order of 10^{-15} s. Thus, for the process to be limited by the reaction itself, the carrier diffusion time for reaching the center from the matrix needs to be shorter than or at least comparable to $\sim 10^{-15}$ s. To travel from the Si matrix to the recombination center, an excess electron will diffuse, on average, half the distance between two centers. Considering that the electron diffusivity is $\sim 25\ \mathrm{cm^2\,s^{-1}}$, a concentration of $3\times 10^{19}\ \mathrm{cm^{-3}}$ evenly distributed centers will be required to give rise to such a short diffusion time. Since neither the precipitates, typically of a density of less than $10^{12}\ \mathrm{cm^{-3}}$, nor the dissolved impurity atoms, typically of a density of less than $10^{17}\ \mathrm{cm^{-3}}$, have such a high concentration, we see that the recombination events should be limited by the diffusion process of electrons to reach the centers. Now, consider only one kind of recombination centers (dissolved atoms or precipitates) with concentration C. Let each center be surrounded by a spherical diffusion domain of radius

$$R=\left(\frac{4}{3\pi C}\right)^{1/3} \tag{11}$$

within which the minority carriers (electrons) diffuse to this recombination center. The *virtual* surface of this recombination center has a spherical shape with a radius determined by the capture cross section via

$$r_{\mathrm{rc}}=\left(\frac{\sigma}{\pi}\right)^{1/2}. \tag{12}$$

Every nonequilibrium minority carrier that reaches the virtual surface of the recombination center recombines. Thus, the excess concentration of minority carriers vanishes at the recombination center, i.e., $\delta n(r)=0$ at $r=r_{\mathrm{rc}}$. Note that the domain size R is much smaller than the thickness of the wafer d_{Si}, then in steady state at $r=R$, $\delta n(r)=\delta n_0=\mathrm{const}$ holds. The distribution of minority carriers in the diffusion domain is described by the diffusion equation in spherical coordinates, with the solution

$$\delta n(r)=\delta n_0\left(1-\frac{r_{\mathrm{rc}}}{r}\right), \tag{13}$$

taking into account that $r_{\mathrm{rc}}\ll R$. The total number of nonequilibrium minority carriers in the domain is $\delta N\approx\delta n_0/C$. The flux density of minority carriers at the lower boundary $r=r_{\mathrm{rc}}$ is found as

$$j(r_{\mathrm{rc}})=-D\left(\frac{d\,\delta n}{dr}\right)_{r_{\mathrm{rc}}}=-D\,\frac{C\,\delta N}{r_{\mathrm{rc}}}. \tag{14}$$

Then

$$\frac{d\,\delta N}{dt}=4\pi r_{\mathrm{rc}}^2\,j(r_{\mathrm{rc}})=-4\pi r_{\mathrm{rc}}DC\,\delta N. \tag{15}$$

On the other hand, by the definition of the recombination constant, we have

$$\frac{d\,\delta N}{dt}=-\alpha_{\mathrm{rec}}\delta N. \tag{16}$$

Combining Eqs. (9), (15), and (16) we obtain the capture cross section for recombination centers of one particular type as

$$\sigma^{\mathrm{eff}}=\frac{4\pi D r_{\mathrm{rc}}}{v_{\mathrm{th}}}. \tag{17}$$

In Eq. (1) the superscript eff specifies that the capture cross section of a recombination center is an effective quantity, which takes into account that near the surface of a recombination center the excess minority carriers are depleted, and the recombination rate is limited by diffusion of these carriers. If the recombination center is a single dissolved metal impurity atom, $r_{\mathrm{rc}}=\beta r_{\mathrm{at}}$, where r_{at} is the atomic size, and $\beta\sim 1$ holds. For a spherical precipitate of radius r_{ppt}, $r_{\mathrm{rc}}\sim r_{\mathrm{ppt}}$ holds. The capture cross section of a single atom is σ_{sol}, and that for a precipitate is then

$$\sigma_{\mathrm{ppt}}=\sigma_{\mathrm{sol}}\frac{r_{\mathrm{ppt}}}{\beta r_{\mathrm{at}}}. \tag{18}$$

The fact that the precipitate capture cross section is proportional to the precipitate radius, rather than its second power, accounts for the diffusion limited recombination process. To further check whether the assumption that carrier recombination is limited by the excess minority carrier diffusion process, we estimate the minority carrier lifetime in the presence of precipitates capable of providing infinitely high recombination rate. If the lifetime turns out to be too short, then the assumption is not valid. Using Eqs. (9) and (18), $v_{\mathrm{th}}=10^5$ m/s, $r_{\mathrm{ppt}}=10$ nm, $r_{\mathrm{at}}=1.7$ Å, and $C_{\mathrm{ppt}}=10^{11}\,\mathrm{cm}^{-3}$, obtain carrier lifetime $\tau=1/\alpha=18\,\mu$s, which is a rather large value. Thus, the diffusion limited recombination assumption does not contradict experimental lifetime results. Equation (18) allows us to evaluate the recombination constant due to the presence of both dissolved and precipitated impurities.

IV. NUMERICAL MODELING OF GETTERING PROCESS

The impurity gettering process involving precipitate dissolution is modeled for the case of using a layer of Al–Si liquid (LAL) on the backside of a Si wafer and Fe as an impurity. The approach can be easily adopted for modeling of any other interstitially dissolved impurities. The thickness of the wafer is assumed to be 200 μm, the thickness of LAL is assumed to be 2 μm, and Fe solubility limit in the LAL is assumed to be 1 at. %, which is an underestimate. The used Fe solubilities and diffusivities are[10]

$$C^{\mathrm{eq}}=1.82\times 10^{26}\exp\left(-\frac{2.94\,\mathrm{eV}}{k_BT}\right)\mathrm{cm}^{-3}, \tag{19}$$

$$D=1.3\times 10^{-3}\exp\left(-\frac{0.68\,\mathrm{eV}}{k_BT}\right)\mathrm{cm}^2\,\mathrm{s}^{-1}, \tag{20}$$

respectively. As initial conditions, the total concentration of Fe atoms in Si, including those in dissolved state and those present in precipitated form, is assumed to be equal to the thermal equilibrium Fe concentration at a (higher) *saturation* temperature T_{sat}, at which the Si wafer was saturated with Fe. The concentration of dissolved Fe in the Si matrix is assumed to be equal to the thermal equilibrium Fe concentration at a (lower) *precipitation* temperature T_{ppt}, at which the Fe precipitation process has taken place to completion, yielding a precipitate density C_{ppt}. The precipitates-Si interfacial energy is assumed to be small and hence neglected. The actual energy of the interface is positive, and dissolution of precipitates should therefore be slightly faster than predicted, and precipitation should be slightly slower. However, this difference is noticeable only at very small precipitate sizes, and does not significantly affect the results obtained for larger precipitates since the role of the interfacial energy decreases as the precipitate size increases. It is also assumed that precipitates are composed of only Fe and Si atoms without a third element, e.g., O or C.[11] The presence of a third element may make the precipitate more stable than pure silicide precipitates, which can further slow down the precipitate dissolution process.

First, time-dependent profiles of Fe concentration and precipitate sizes throughout the wafer were calculated using Eqs. (3)–(7). The results then allow us to calculate the relative integrated recombination constant α^* as defined by Eq. (10). The reciprocal value of α^* is the relative lifetime after and before the gettering process. The quantity α^* is calculated at each instant with respect to α_{rec} at the beginning of the process. It provides an instantaneous monitoring of the impurity concentration and distribution between solution and precipitates at any time during the gettering process, as would be observed if the process was abruptly terminated by quenching the sample from the gettering temperature down to room temperature. It is specifically noted that the calculated recombination constant is that of the considered impurity only. In experiments, there are other recombination centers and impurities in the crystal also contributing to the observed recombination rate.

Gettering of precipitated impurity requires a significantly longer time than that of dissolved impurity atoms since precipitates continuously supply impurity atoms into the solid solution until they are completely dissolved. An example of the calculated profiles of dissolved impurity concentration and diameter of precipitates at different stages of the gettering process is shown in Fig. 1. The getter layer is deposited on the side corresponding to zero depth. If the precipitation temperature T_{ppt} is lower than the *gettering* temperature T_{get}, after the onset of the gettering process, C_{sol} increases and reaches its thermal equilibrium value at T_{get} because the rate of precipitate dissolution exceeds the rate of impurity outdiffusion to the LAL layer. This causes a temporary increase in α^*. Then, at a given depth x, C_{sol} remains almost the same until precipitates at that depth are completely dissolved. The dissolution of precipitates proceeds in a layer by layer manner, starting at the LAL–Si interface. After all precipitates are dissolved, C_{sol} is rapidly reduced to the value determined by the segregation coefficient between LAL and Si. Only at this point does the value of α^* decrease to become lower than its initial value, see the solid line case of Fig. 2. The experimentally observed recombination constant strongly depends on the gettering time and cooling rate, which determines the balance of impurity between solid solution and precipitates. If the gettering process is not conducted long enough to dissolve all precipitates, and the sample is cooled sufficiently fast, the measured value of α^* may exceed its initial value. Moreover, under certain conditions, α^* can increase after the gettering process, irrespective of the gettering time used. For instance, for the case of $T_{\mathrm{sat}}=1000\,°\mathrm{C}$, $T_{\mathrm{ppt}}=600\,°\mathrm{C}$, and $C_{\mathrm{ppt}}=10^{10}\,\mathrm{cm}^{-3}$, gettering conducted at 1200 °C for a sufficiently long time to reach the equilibrium

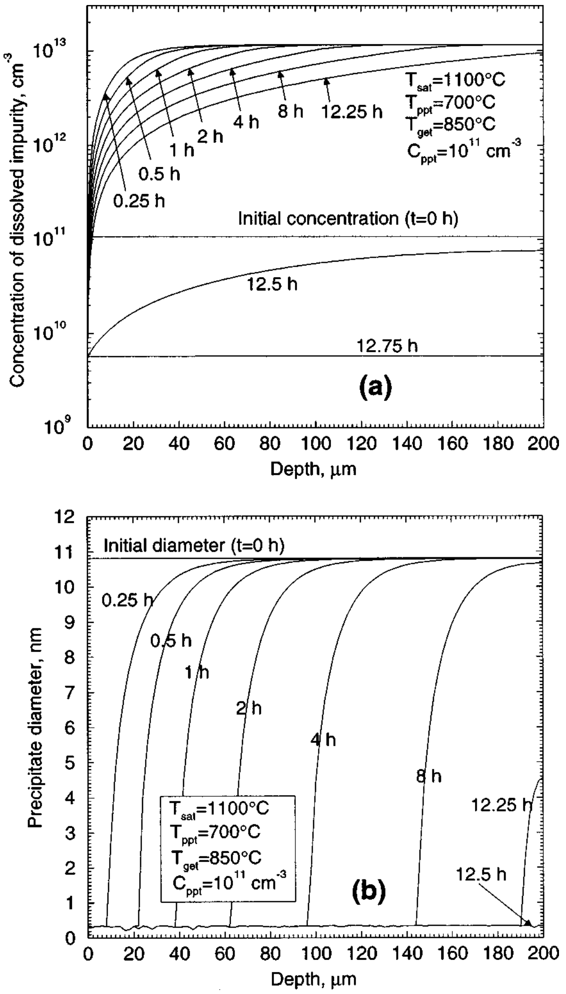

FIG. 1. Calculated concentration profiles of dissolved Fe (a) and precipitate radii (b) at different stages of the gettering process. The gettering Al–Si liquid layer is located at 0 depth.

state, leads to an increase of α^* by a factor of 3. This is understood by considering that, although the total concentration of Fe is much lower after gettering, most Fe atoms are in solution, and are much more active electrically. This explains the fact that the carrier lifetime may drop as a result of impurity gettering in multicrystalline Si.[5,6] If $T_{\mathrm{ppt}}>T_{\mathrm{get}}$, the concentration of dissolved impurity drops at the beginning of the gettering process, and precipitates grow. This results in a decrease of α^*, as shown in Fig. 2. Such a process is similar to the effect of intrinsic gettering. Just by itself, it is of limited benefit for practical applications because usually T_{ppt} can be expected to be fairly low for an as-grown crystal, and the needed T_{get} will be so low that a desired result will not be obtained in a reasonable gettering time duration.

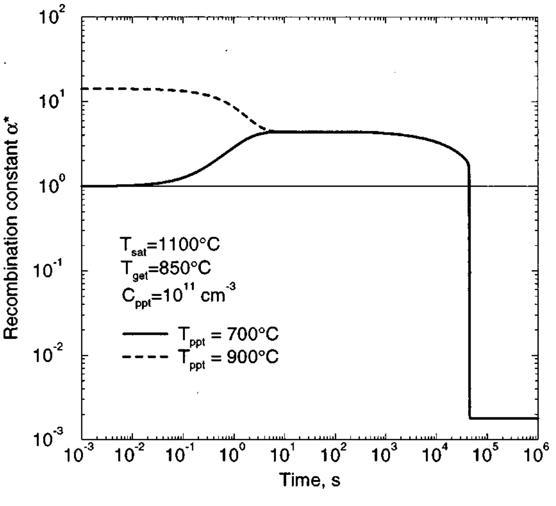

FIG. 2. Relative integrated recombination constant as a function of gettering times. Normalization is made to the value at the beginning of the process shown by the solid line.

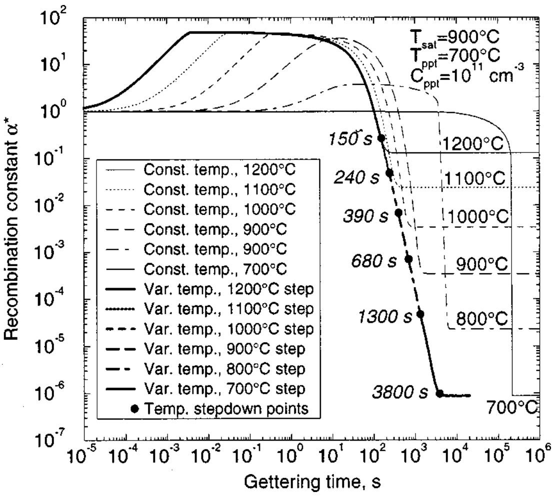

FIG. 3. Calculated relative integrated recombination constant as a function of gettering times for different gettering temperatures. The light lines correspond to constant temperature processes. The heavy line corresponds to a variable temperature process with temperature decreased from 1200 to 700 °C in 100 °C steps, at the indicated temperature steeping-down points.

The time needed to complete the gettering process and to reach equilibrium depends on the initial concentration of impurity, precipitate size and density, and the process temperatures. At higher T_{get}, the needed time is shorter but, on the other hand, the residual concentration of dissolved impurity is higher, which leads to a larger ultimately attainable α^* value, see the light lines in Fig. 3. For instance, at 1200 °C, the process is completed in about 200 s, but the reduction in α^* is comparatively small. On the other hand, gettering at 700 °C provides a very significant decrease in α^*, but requires 55 h of gettering time. Thus, the choice of a gettering temperature is an inevitable compromise between the process duration and the attainable reduction in the recombination constant.

We suggest a variable temperature process so as to take advantage of both the high and low temperature processes: short gettering time and small recombination coefficient. A high gettering temperature stage is employed first to dissolve the precipitates and to rapidly outdiffuse the dissolved impurities to the LAL. Subsequently, a lower temperature gettering stage is implemented to reduce the dissolved Fe concentration to attain a low α^* value. For the purpose of further shortening the gettering time, a multistage process has been considered, see the heavy curve in Fig. 3. For this case, the temperature is decreased from 1200 to 700 °C in 100 °C steps. As a result, the large recombination constant decrease

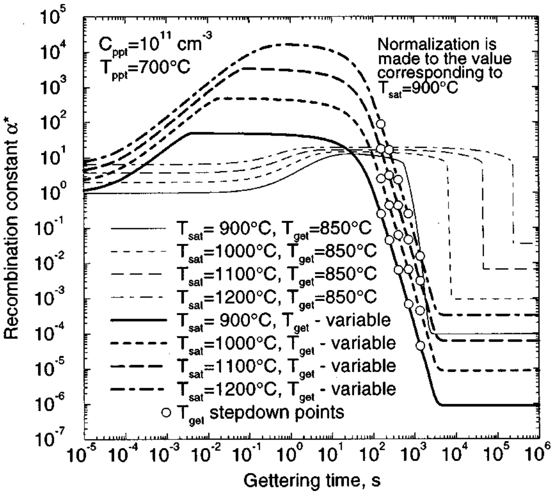

FIG. 4. Calculated relative integrated recombination constant as a function of gettering times for different initial impurity saturation temperatures. The light lines correspond to constant temperature gettering conducted at 850 °C. The heavy lines correspond to variable temperature processes with temperature decreased from 1200 to 700 °C in 100 °C steps at the indicated temperature stepping-down points. Variable temperature processes were optimized for gettering times.

attainable for the 700 °C gettering process, which needed 55 h of gettering time at a constant temperature, is achieved in ~1 h. Continuous ramping down of the gettering temperature can shorten the gettering time slightly more. Another highly significant advantage of the variable temperature gettering is that the optimum temperature regime is almost independent of the initial impurity concentration and distribution between the solution and precipitates. In Fig. 4, results of modeled constant temperature and variable temperature gettering processes are compared for different T_{sat}. The variable temperature processes are optimized for gettering time, and the optimum temperature regime appears to be almost independent of T_{sat}, as long as the starting gettering temperature exceeded T_{sat}. As the modeling results show, it is also independent of T_{ppt}. In all cases, constant temperature processes either require much longer gettering times or provide less reduction of recombination constant at all stages of the gettering process, except for the very early onset stage, which is of no practical importance. The benefits of the variable temperature gettering process are especially noticeable at higher T_{sat}, i.e., with larger impurity concentrations, which are typical for low cost MC Si. Variable temperature gettering may also be very beneficial for gettering of impurities from precipitates containing O or C,[10] since such precipitates may be especially slow to release the impurity.

V. CONCLUSIONS

Physical and numerical modeling of the processes of gettering precipitated metallic impurities (Fe) from Si bulk has been carried out employing the gettering method of using a liquid Al–Si layer. The results of the gettering are evaluated using a *relative integrated recombination constant*, which accounts for minority carrier recombination events at both precipitates and at individual dissolved impurity atoms throughout the Si wafer. The effective capture cross section of precipitates is proportional to the cubic root of the number of atoms in them. This explains the low electrical activity of impurities in precipitates. During gettering, precipitates have to be completely dissolved before recombination coefficient can be reduced. This requires either long process time, or high temperature resulting in high residual impurity concentration. Thus, gettering at a constant temperature is an inevitable compromise between very long process time at lower gettering temperatures and high residual concentration of impurity at high gettering temperatures. A variable temperature gettering process is proposed. This process allows us to take advantage of the large gettering rate of the high temperature processes for shortening of the needed gettering times and the attainable low residual impurity concentrations of the low temperature process.

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