A Novel Approach for the Evaluation of a Phosphorus Diffusion Design of Experiment

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Abstract. The emitter formation in industrial p-type silicon solar cells is generally done by phosphorus diffusion. To optimize the emitter in terms of high efficiency, series resistance and recombination losses of the emitter are balanced out. In this work, we present the results of a design of experiment (DoE) to optimize the main parameters of the P-diffusion. Therefore, we use a novel approach to evaluate the results of the DoE: We approximate the unavoidable correlation between the emitter saturation current density (j_{0e}) and the emitter sheet resistance (ρ_{sh}) and create a new target variable (dj_{0e}), which describes the deviation from this correlation. This allows us to understand the key parameters that can minimize emitter saturation current density while keeping emitter sheet resistance at a target value.

INTRODUCTION

The phosphorus diffusion is a key step in the industrial p-type silicon solar cell production [1]. Generally, the source of the phosphorus is phosphosilicate glass (PSG), which is formed by the reaction of phosphoryl chloride ($POCl_3$) and oxygen with the silicon wafer in a furnace. This process step is called PSG deposition (PD). Subsequently, P is diffused into the silicon wafer during a step called drive-in (DI). The higher the phosphorus concentration, the lower is the sheet resistance. However, a higher phosphorus concentration increases Shockley-Read-Hall (SRH) and Auger recombination. If the phosphorus concentration is well above the solubility limit of about 1×10^{20} cm^{-3} the concentration of electrically inactive phosphorus increases SRH recombination [2]. If the phosphorous concentration is lower, a further reduction of the phosphorus [3,4,5] minimizes Auger recombination while the recombination velocity at the emitter surface needs to be minimized as well to maintain good surface passivation [6]. Additional effects, as gettering and change of the bulk carrier lifetime during the diffusion process influences the total recombination [7]. This leads to a very complex optimization task.

EXPERIMENTAL DETAILS

The diffusion experiments are carried out in a Centrotherm diffusion furnace. We systematically varied seven process parameters using a circumscribed central composite design of experiment [8]: deposition temperature, deposition time, deposition oxygen flow, deposition $POCl_3/N_2$ flow, drive-in temperature, drive-in time, and drive-in oxygen flow. This results in 85 experimental setups. The minimum and maximum values as well as the central point are listed in Tab. 1.

For the determination of the emitter saturation current density j_{0e} high-ohmic Cz-Si wafers are used which are textured, diffused and passivated identically on both sides and finally fired in a belt furnace. j_{0e} is derived using the procedure of Kane and Swanson [9] in combination with the quasi-steady state photoconductance (QSSPC) method

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[10]. For the evaluation the Richter Auger model and Band-gap narrowing (BGN) is used [11], i.e. the effective intrinsic carrier density depends on the boron doping concentration.

TABLE 1. Minimum and maximum values and the central point of the circumscribed central composite design of experiment [8]. Values are given for the phosphorus deposition (PD) and the drive-in (DI) step.

	PD phi($POCl_3/N_2$) (sccm)	PD phi(O_2) (sccm)	PD T (°C)	PD t (min)	DI phi(O2) (sccm)	DI T (°C)	DI t (min)
minimum value	245	165	820	10	1000	820	10
maximum value	505	335	860	30	2000	860	30
central point	375	250	840	20	1500	840	20

RESULTS

Figure 1 shows the resulting values with the well-known correlation between the emitter sheet resistance ρ_{sh} and the emitter saturation current density j_{0e}. We approximate this correlation by an empirical quadratic function. The vertical deviation from this function results in our new target variable (dj_{0e}). Therefore, a positive value of dj_{0e} mean, that the j_{0e} is lower than expected from the empirical correlation.

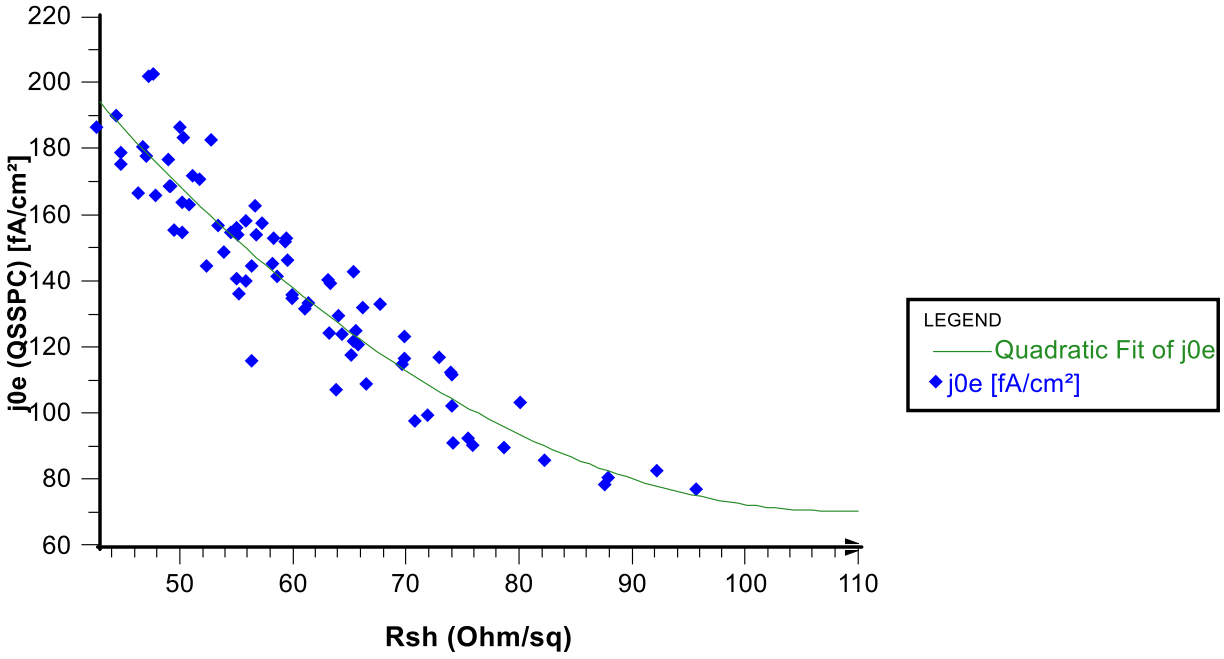

FIGURE 1. Resulting correlation between j_{0e} and ρ_{sh} with an empirical quadratic fit function.

Subsequently, we analyze the results of the DoE by building a second-order response surface model (RSM). That means we express the dependencies between the input variables (see Table 1) and the output variables (dj_{0e}, ρ_{sh}) with a second-order polynomial expression (including linear, quadratic and interaction terms) [8]. This RSM allows optimizations under various boundary conditions. As an example, we show between Fig. 2 and Fig. 3 the optimization of the diffusion parameters (green lines) towards a lower j_{0e} while keeping the ρ_{sh} constant at 90 Ω/sq.

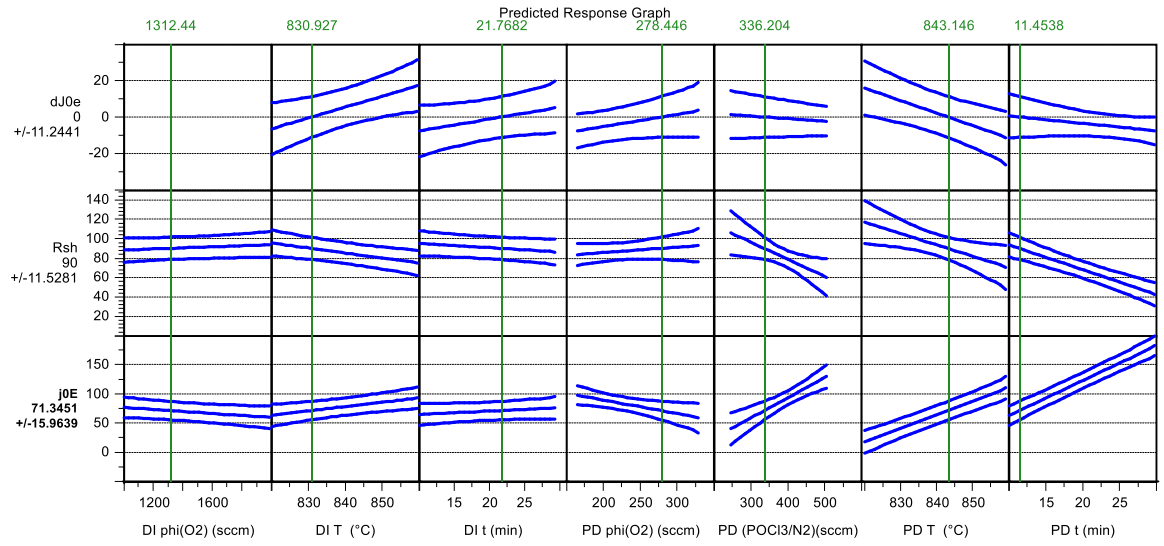

FIGURE 2. RSM – Predicted Response for the non-optimized diffusion parameters (green lines and green values) with ρ_{sh} constant at 90 Ω/sq. Expected j_{0e} = 71 fA/cm^2.

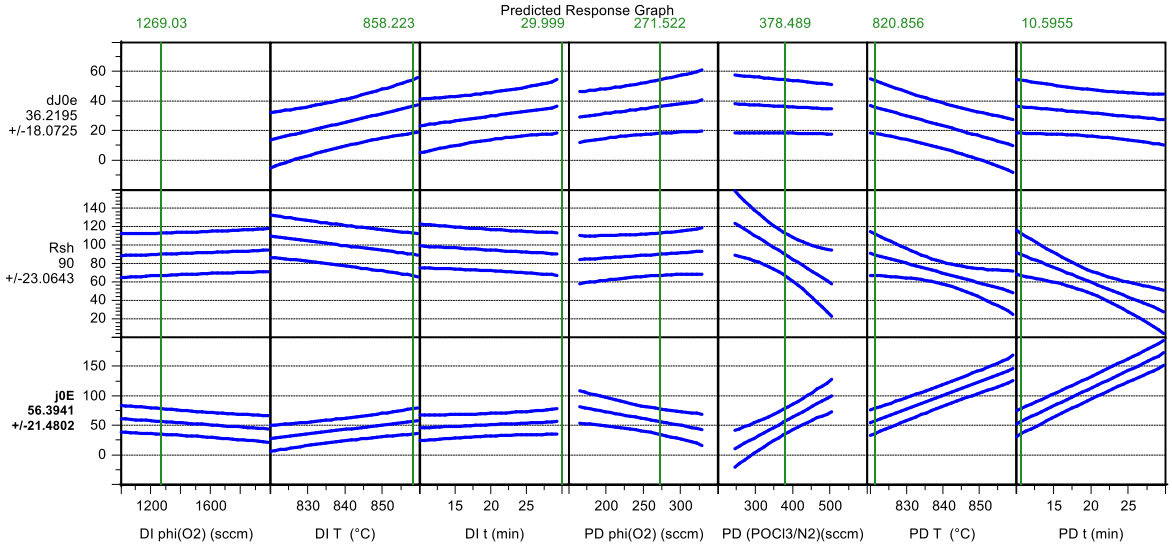

FIGURE 3. RSM – Predicted Response for the optimized diffusion parameters (green lines and green values) with ρ_{sh} constant at 90 Ω/sq. Expected j_{0e} = 56 fA/cm^2.

DISCUSSION

The main effect that reduces j_{0e} while keeping the ρ_{sh} constant is the increase of the drive in (DI) temperature/time and the reduction of the deposition (PD) temperature. This can be seen by looking at the slope of the dj_{0e} curve (Figure 2 and 3, blue curve dj_{0e}) versus DI T, DI t and PD T. The main physical explanation is the different ratio between electrically active and inactive phosphorus [2]. The inactive phosphorus increases the recombination (j_{0e}) without an influence on the emitter sheet resistance ρ_{sh}. The phosphorous concentration also

affects the Auger recombination and the recombination velocity at the emitter surface passivation. We assume that we have enough phosphorus in the PSG that can diffuse into the wafer during the whole process time. However, the high oxygen flow during the DI may oxidize the silicon surface and form a barrier that reduces the diffusion of phosphorus from PSG into the wafer. Additional effects (e.g. gettering) are also likely to influence dj_{0e}. Hence, there are also some not-so-obvious dependencies, as for example a strong interaction term between the PD oxygen flow and the PD temperature, which cannot be easily explained within a physical diffusion model. The DoE approach we described in this study, builds an empirical model of the process. This empirical model allows optimization within the boundaries of the input variables. However, the DoE approach with the new target variable (dj_{0e}) allows an efficient optimization of this very complex diffusion process for different goals (e.g. optimized emitter surface passivation) and towards much lower j_{0e} values. This approach has been successfully applied to an industrial production diffusion process in the past [12].

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