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Computer Simulations of Edge Effects in a Small-Area Mesa N-P Junction Diode

Preprint

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Computer Simulation of Edge Effects in a Small-Area Mesa N-P Junction Diode

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ABSTRACT

The influence of edges on the performance of small-area solar cells is determined using a modified commercial, finite-element software package. The n^+/p mesa device is modeled as having a sub-oxide layer on the edges, which acquires positive charges that result in development of an electric field within the device. Our computer simulations include generation/recombination at the diode edges as well as the influence of light on the recombination characteristics of the edges. We present a description of our model, dark and illuminated characteristics of devices with various surface charge concentrations, and the dynamics of carrier generation/recombination. The influence of edge geometry on diode performance is determined.

INTRODUCTION

Use of mesa diode arrays, fabricated by chemical etching, is a valuable technique for detailed characterization of photovoltaic properties of single-crystalline and multicrystalline silicon wafers. The chemical etching process creates a sub-oxide, which is rich in hydrogen and passivates the edges. The diode array consists of 100-mil-diameter devices that are etched 3 to 4 microns deep and have a blanket back Al contact common to all devices. Each device has a front Al contact, 10 mils in diameter, for ease in automatic probing. The diodes are electrically isolated from one another and can be probed to measure the current density versus voltage curves under dark and illuminated conditions [1,2]. We find that the degree of passivation depends strongly on the process conditions. To understand the details of the edge passivation, we modeled an n-p junction diode using a commercial, finite-element software package. These simulations have led to a determination of the self-consistent solution to the continuity equations for electrons and holes using the steady-state drift-diffusion model for carrier dynamics coupled with electric potential determined from Poisson's equation [3]. The purpose of these simulations is to determine the influence of edge conditions on the overall performance of mesa diodes under dark and illuminated conditions. In particular, we examine the effect of edge shape on the I-V characteristics of the diode.

The underlying mechanisms of bulk and surface recombination have been well established for crystalline silicon semiconductor devices [4-7]. We have applied them to our mesa device using the COMSOL software. Our simulations show that the space-charge region becomes extended along the vertical edge of the mesa diode due to the fixed positive surface charge. At the intersection of the vertical edge and step, a strong electric field is produced because it has a small convex radius of curvature [8]. Depending on the sharpness of this intersection, the entire device can become significantly shunted. Simulations have been performed with a sharp corner and a smooth curve at the intersection of the vertical edge and the step. The use of a smooth

curved transition results in significantly lower dark current density versus voltage and a greater open-circuit voltage and fill factor under illumination. Yet, even with a curved transition, the space charge region can extend approximately 100 microns into a 199.5-micron-thick mesa diode and have a bulk recombination rate that is two orders of magnitude greater than the rest of the device at low forward biases.

SIMULATION RESULTS

The diode configuration used for modeling is illustrated in Figure 1. Each diode is 100 mils in diameter, etched 3.5 mils deep, and has a concentric front metallization of 10 mils. The surface of the diode is coated with an antireflection layer having an interface charge of $1x10^{11}$ cm^{-2}. In the current simulation, we assume that the edge of the diode has a thin oxide, and the charge density of the oxide is varied from $1x10^{11}$ cm^{-2} to $5x10^{11}$ cm^{-2}. The junction depth is assumed to be 0.5 μm.

The mesa diode was simulated under dark and illuminated conditions. Figure 1 shows a cross section of the device. Detailed simulations have shown that charge loss can occurs via a number of mechanisms, which include: carrier flow from the diode to the edge, recombination by the field produced at the edge, which propagates radially into the diode and through the thickness of the diode, and recombination at the etched surface.

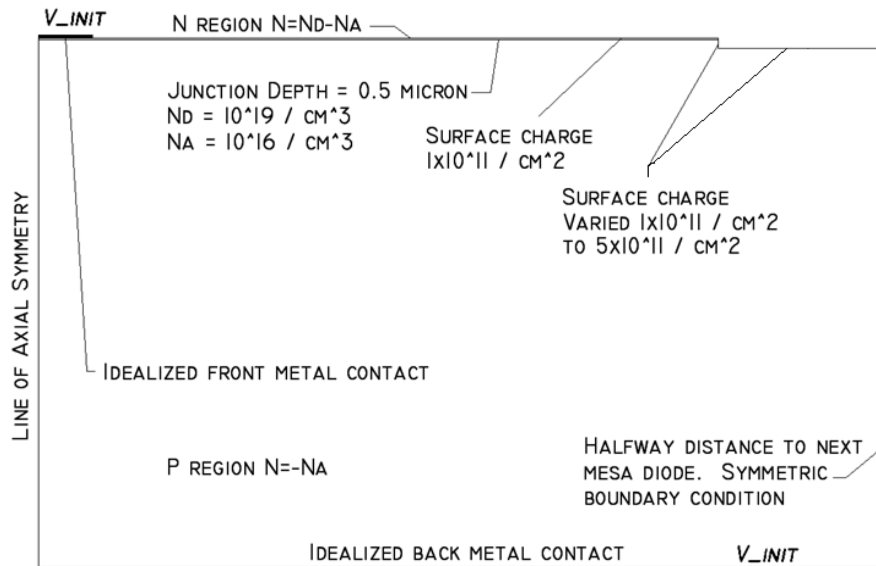

Figure 1. Cross section of modeled mesa diode with bulk and surface conditions

Dark Condition

The dark current density versus voltage plots of the simulations are shown in Figure 2. The current density increases with increasing surface charge. The initial increase in dark current density is due predominantly to recombination near the mesa's edge. The greatest increase occurs at low voltages and is due to resistive shunting, which is related to the distortion of the electric field at the edge of the mesa. One of the most important results of the simulations performed on the mesa diode is the calculation of a high point in the electric field at the corner of the vertical edge and the step. The resultant current density versus voltage curves for the

simulations in Figure 2 were performed with a corner that was a right angle with a sharp point. To determine if this feature of the mesa diode was responsible for the increase in dark current density, similar simulations were run with a curved transition rather than a sharp corner. A small, curved piece of p-type semiconductor was added at the corner of the vertical edge of the mesa and the step. It was defined as a second-order Bezier curve with a height and length of 3.5 μm. This height was chosen because the junction is 3.5 μm above the step. The bulk

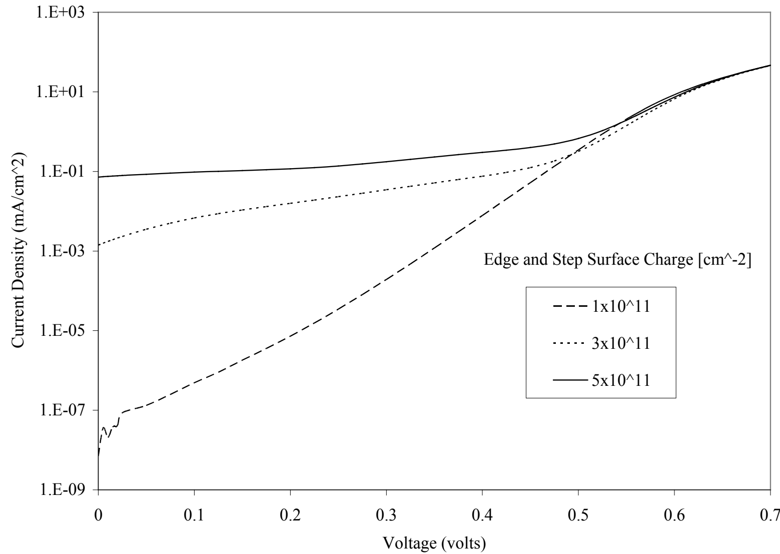

Figure 2. Dark current density vs. voltage for the mesa diode at different vertical edge and step surface charges

recombination rate and electric field for simulations with the vertical edge and step surface charges of $5x10^{11}$ cm^{-2} are shown for sharp and curved corners in Figure 3. The addition of a curved piece at the mesa's edge clearly reduces the bulk recombination rate in this region. However, the curved piece has a smaller radius of curvature than the flat continuous sections away from it. Therefore, even with an additional curved piece, the bulk recombination rate

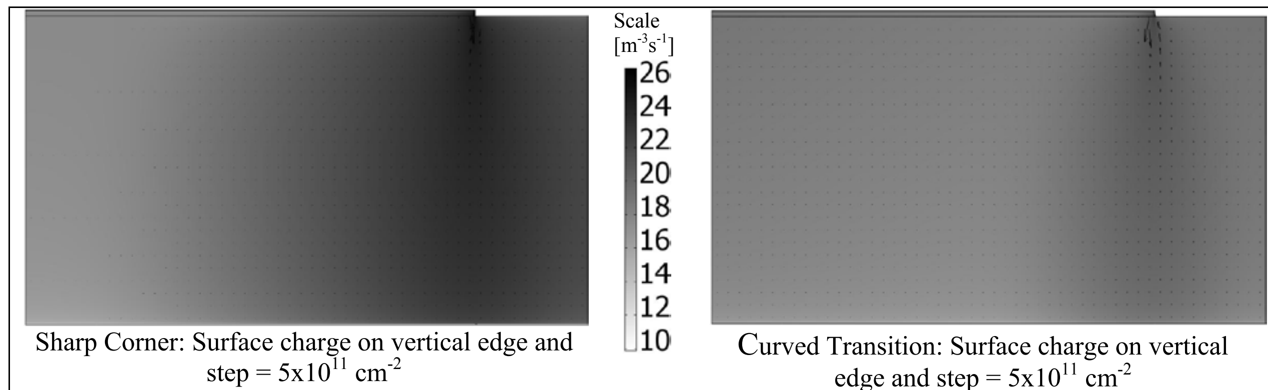

Figure 3. Comparison of bulk recombination rate (logarithmic) and electric field at 0.1 volt forward bias for a mesa diode with sharp and curved corners with a surface charge of $5x10^{11}$ cm^{-2} under dark conditions.

and electric field in this region are greater than the rest of the device except for the junction, where they are almost equal. Consequently, the results of the dark simulations of the mesa diode indicate that the distortion of the electric field at the corner of the junction and the vertical edge, and the step and the vertical edge in conjunction with the inversion layer on the p-side adjacent to the junction, results in an extension of the space-charge region deep into the bulk of the device. This leads to an increase in the recombination rate and the dark current, particularly at low forward biases.

A comparison of the dark-current density versus voltage for sharp and curved corners is shown in Figure 4 for a surface charge of $5x10^{11}$ cm^{-2}. By increasing the radius of curvature of corner at the step and vertical edge, the resistive shunting caused by excessive bulk recombination can be reduced significantly. For a surface charge of $5x10^{11}$ cm^{-2}, the reduction of dark current density is almost four orders of magnitude at low forward biases.

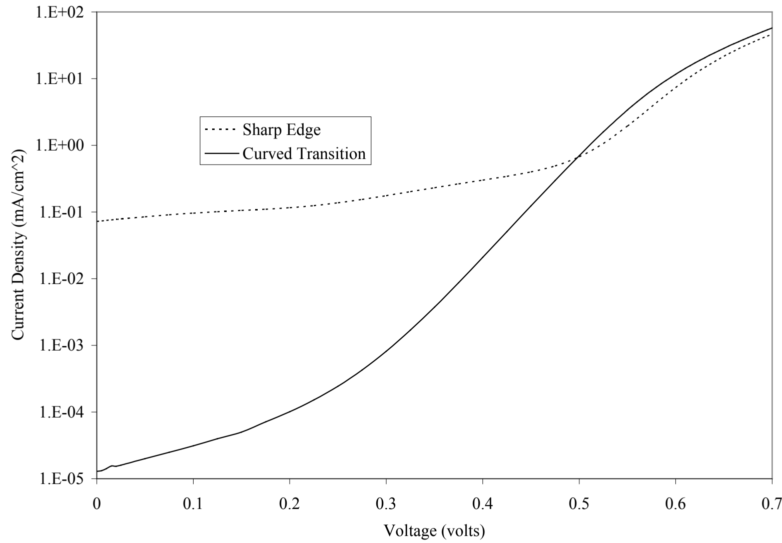

Figure 4. Current density vs. voltage plots of the comparison of sharp and curved transitions between the step and the vertical lines with a surface charge of $5x10^{11}$ cm^{-2} under dark conditions.

Illuminated Condition

Simulations of the mesa diode were also performed under illuminated conditions, in which only the vertical-edge surface charge was changed from $1x10^{11}$ cm^{-2} to $5x10^{11}$ cm^{-2}. The resulting illuminated current density versus voltage curves are shown in Figure 5. The open-circuit voltage and fill factor become reduced as the vertical-edge surface charge is increased from $1x10^{11}$ cm^{-2} to $5x10^{11}$ cm^{-2}. The loss in V_{oc} and FF are significant, and the mechanism that causes them as the charge increases is a result of increased recombination due to the increased electric field caused by the sharp corner at the edge of the mesa.

To determine if the sharp corner at the edge of mesa was the cause of the reduction in open-circuit voltage and fill factor, simulations under illumination were performed with a curved piece at the corner of the vertical edge and the step. It had exactly the same dimensions as the one used for the dark simulations. Also, the simulations using a sharp corner were repeated with the surface charge of the vertical edge and the step set to the same value.

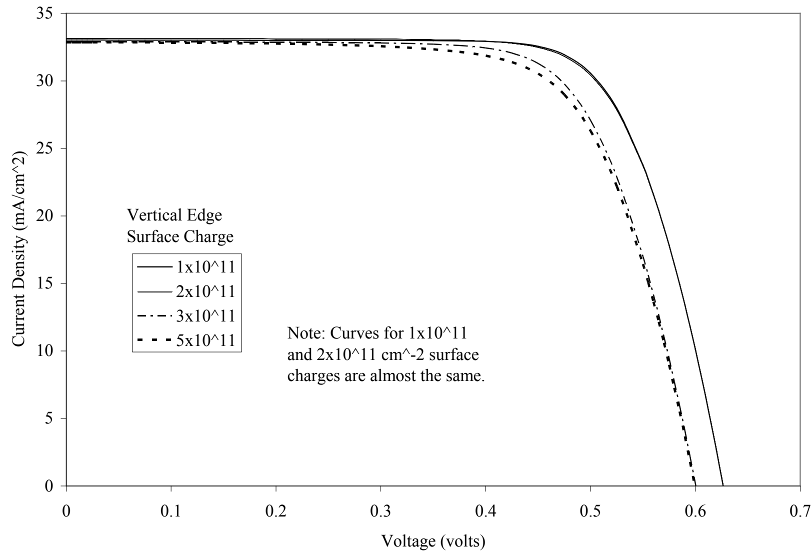

Figure 5. Illuminated current density vs. voltage for the mesa diode at different vertical edge charges.

The illuminated current density versus voltage plots for simulations performed with a sharp corner and a curved transition with a surface charge of $5x10^{11}$ cm^{-2} are shown in Figure 6. The simulation with a curved transition has a greater open-circuit voltage and fill factor. This occurs because there is a lower recombination rate in the mesa diodes modeled with a curved transition. It should be noted that the short-circuit current (J_{sc}) values for the simulations shown in Figure 6 are significantly greater than the J_{sc} values shown in Figure 5; this is because the surface charge was increased on the step adjacent to the mesa's edge. This results in an inverted surface, which significantly reduces the recombination rate in this region, and consequently leads to an improved J_{sc} value.

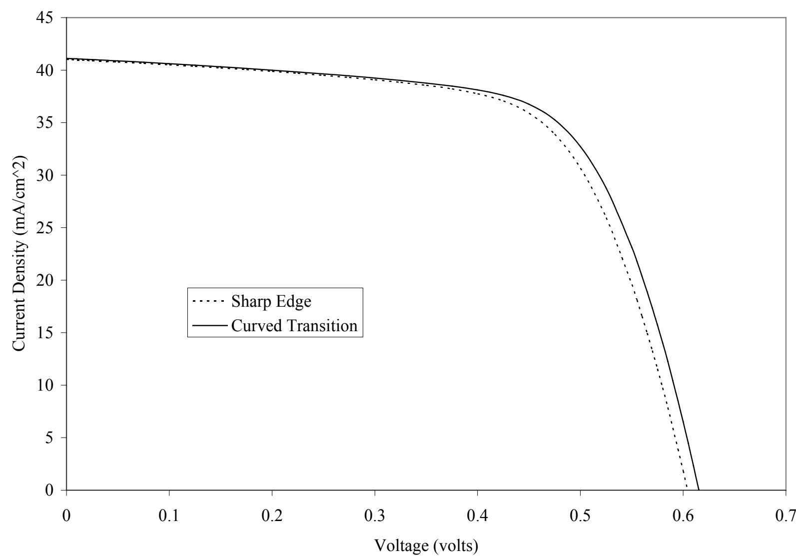

Figure 6. Current density vs. voltage plots of the comparison of sharp and curved transitions between the step and the vertical lines with a surface charge of $5x10^{11}$ cm^{-2} under illuminated conditions.

CONCLUSIONS

The geometric features of the edge of the mesa diode can significantly distort the electric field throughout a large portion of the bulk device. The most important feature occurs at the intersection of the vertical edge and step because an electric field becomes large near areas having a convex radius of curvature and can reach extreme values at sharp points [8]. In certain cases, the distortion can expand the space charge region over hundreds of microns in all directions emanating from the edge. It was shown that changing the interface from a sharp perpendicular step to a Bezier curve in the simulations can greatly reduce the dark-current density and increase the open-circuit voltage and fill factor. This is important because the chemical etch used to delineate the mesa diodes is isotropic and leaves behind a curved transition. Even with a curved interface at the vertical edge and step, the edge effect is a significant source of recombination in the mesa diode, in which the recombination rate can be more than two orders of magnitude greater than the rest of the bulk and this region can extend approximately 100 μm into the device from the curved interface. Therefore, the edge effect in a mesa diode is a result of the space-charge region extending along the vertical edge because of the inverted region on the p-side of the junction, then expanding deep into the bulk device because of the strong electric field at the intersection of the vertical edge and the step. This results in a significant increase in recombination rate throughout the device, an increase in dark-current density, and a reduction in open-circuit voltage and fill factor under illumination.

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