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Solar Energy Materials and Solar Cells 32 (1994) 395–403

Solar Energy Materials and Solar Cells

Donor–acceptor pairs to limit V_{oc}-improvement of photo-diodes

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(Received 21 July 1993)

Abstract

When deep-level centers are inserted near the junction interface, the open-circuit voltage of photo-diodes is reduced. The performance degradation due to the doped layer is sensitively position-dependent; its maximum effect is at a position where $n \simeq p$, for similar recombination rates of electrons and holes. In high-efficient solar cells, it is suggested that donor–acceptor pairs that are created by the conventional diffusion process are responsible for the unintentional limitation of the open-circuit voltage. Computation of the solution curves of transport-, continuity-, and Poisson equations for a two-carrier model indicate that the omission of close pairs by insertion of a thin undoped layer (inverse delta-doping), and consequential reduction in the density of distant pairs causes an increase of the open-circuit voltage and fill factor without concomitant decrease of the short-circuit current.

1. Introduction

Junction recombination is known to degrade the diode performance [1]. Such recombination is the major contributor to a reduction of the open-circuit voltage and fill factor long before it is strong enough to also reduce the saturation current. The reason for the reduction in V_{oc} can be interpreted as an increase in the junction leakage current and caused by the recombination current.

Earlier investigation of an inserted thin sheet with an *increased* density of deeplevel centers (we will call this a "delta-doped layer") show a strong dependency of V_{oc} and the fill factor (FF) on the position of its incorporation with respect to the metallurgical interface of a symmetrically doped *pn*-junction with a

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SSDI 0927-0248(93)E0103-K

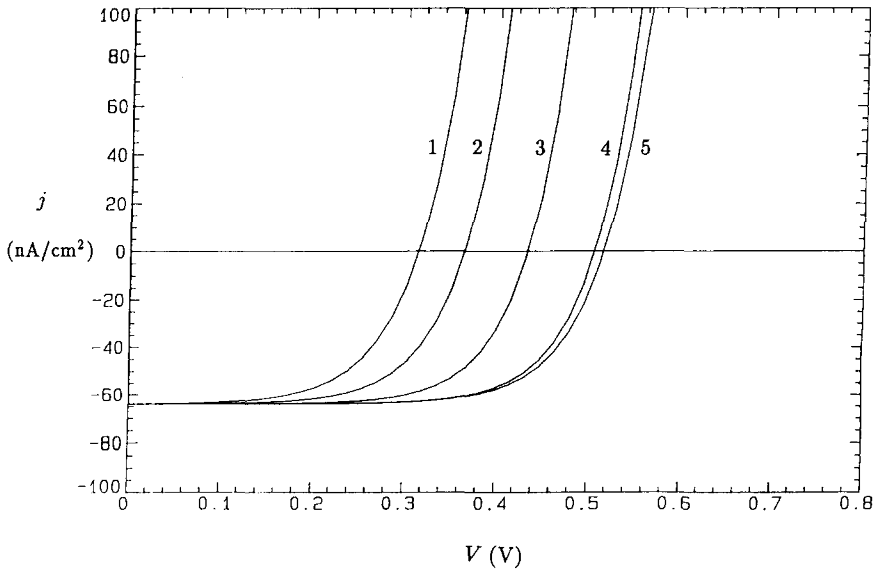

Fig. 1. j–V characteristics of thin symmetrically doped GaAs photodiodes with homogeneous optical generation rates of $g_0 = 10^{16}$ cm^{-3} s^{-1} with delta-doped deep levels at $E_r = E_i$ within a layer of 5 nm thickness, resulting in a minority carrier lifetime within this layer of $\tau = 10^{-9}$ s. The delta-doped sheet is placed at the p-side with the distance from the metallurgical interface of 0, 5, 10 and 20 nm for curves 1–4, respectively. Curve 5 is computed for no delta-doped layer. The carrier lifetime in both sides of the device is assumed as 10^{-7} s (shallow doping 10^{17} cm^{-3}).

total thickness of 400 nm. [1] It causes a significant degradation of V_{oc} and FF only when the delta-doped layer is close to the interface [2] (see Fig. 1).

For the reported numerical results we have integrated transport-, continuity-, and Poisson equations for a two-carrier model using a modified PC-1D software [3]. We used parameters for a typical GaAs homojunction photo-diode, as listed in Refs. [2,4]. Other results of delta-doping that influence the performance of solar cells are listed in ref. [5].

2. Inverse-delta-doping

Based on these results it is suggestive to try the opposite of delta-doping, namely by introducing a thin sheet that is deprived of deep-level defects (we will refer to such a sheet as an "inverse-delta-doped layer").

[1] We are limiting the changes in doping densities between the sheet and its surrounding to values at which the resulting potential well is shallow enough to neglect complications of the level spectrum by quantum well effects [6].

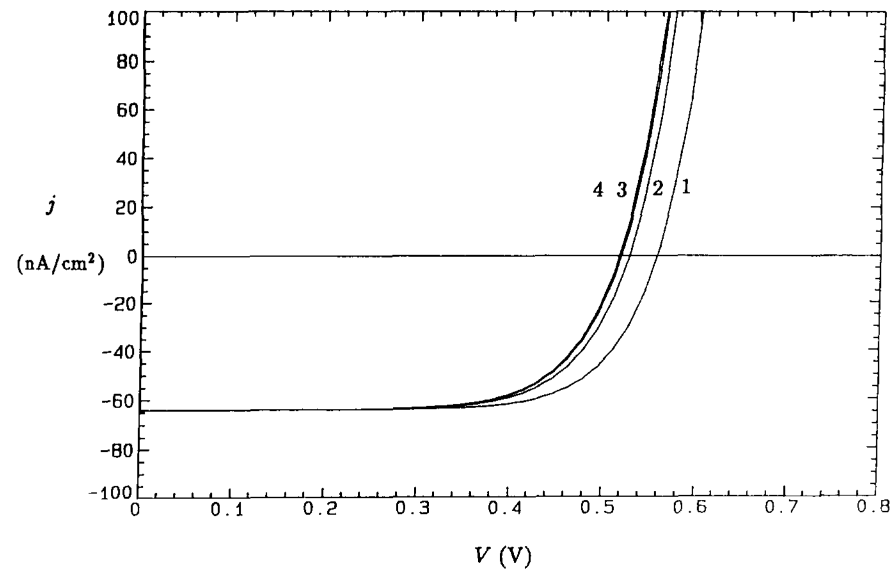

Fig. 2. $j-V$ characteristics as in Fig. 1 however, with an inverse-delta-doped layer of 5 nm thickness and of a substantially reduced density of deep-level centers, resulting in a minority carrier lifetime of $\tau = 10^{-5}$ s. The shift of the center-plane of this sheet from the metallurgical boundary of the *pn*-junction is 10, 5 and 0 nm for curves 3–1, respectively. Curve 4 is computed without an interlayer.

Fig. 2 shows the results for an inverse-delta-doped layer with a factor of 0.01 reduced density of recombination centers. One observes an increase in the open-circuit voltage (and fill factor) when the sheet approaches the interface.

The open-circuit voltage and the fill factor increase with increasing width δ of the layer that retains the appropriate shallow dopant but has a substantially decreased density of deep-level defects acting as recombination centers. This is shown for the V_{oc}-improvement in Fig. 3.

In asymmetrically doped *pn*-junctions the inverse-delta-doped layer must be centered precisely at the position of the cross-over of $n(x)$ and $p(x)$ in order to maximize its beneficial influence. This cross-over is shifted from the metallurgical interface into the lower doped region by a distance on the order of the Debye length [7].

The reason for this sensitivity is caused by the availability of both carriers for recombination at the cross-over [5]. It can be visualized from the distribution of electron and hole currents which show the steepest slope due to recombination losses at the position where $n \simeq p$ (curve 3 shown for the electron current in Fig. 4). The inverse-delta-doped sheet reduces this slope within the sheet to a negligible value as seen for curves 1 and 2 in Fig. 4. The sheet, therefore, has the highest influence of reducing the total loss current when it is located at the position of its steepest slope, as shown for curve 1. Shifting it by only 15 nm from the cross-over in the given example reduces its influence on the total loss current to a negligible value (curve 2 in Fig. 4).

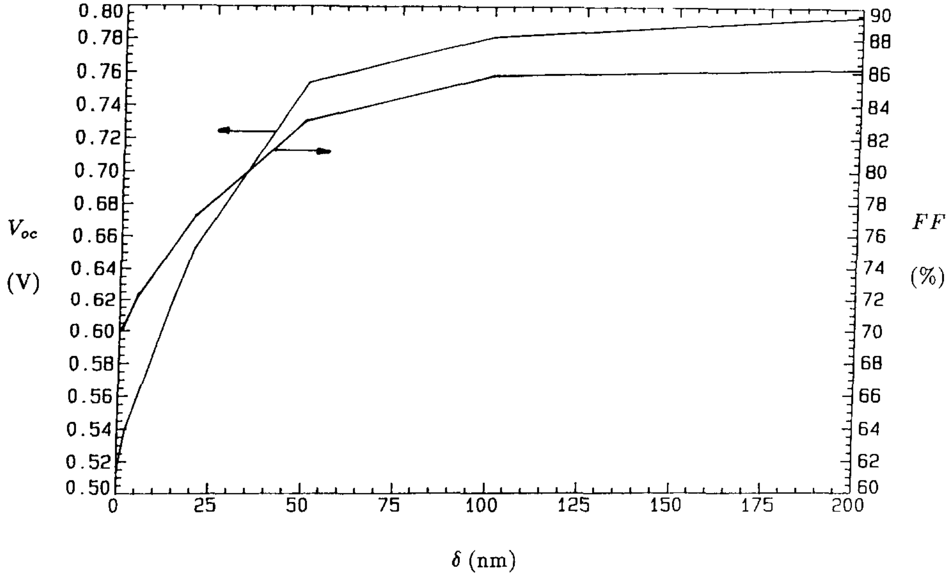

Fig. 3. The improvement of V_{oc} and the fill factor (FF) as a function of the inverse-delta-doped layer thickness δ for the symmetrical *pn*-junction diode as given in Fig. 2. The inserted layer remains centered at the metallurgical boundary and has a minority carrier lifetime of $\tau = 10^{-5}$ s.

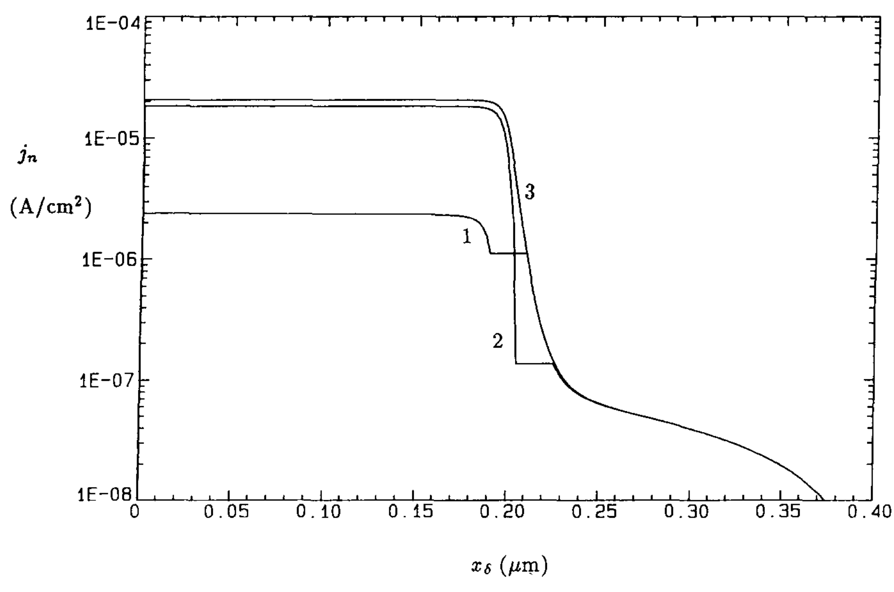

Fig. 4. Dark electron current distribution in the photo diode given in Fig. 2 for an inverse-delta-doped sheet of 20 nm thickness at the metallurgical interface ($x_\delta = 0.2$ μm), 15 nm shifted into the *p*-type region, and with no interlayer for curves 1–3, respectively. The minority carrier life time in the inverse-delta-doped sheet is 10^{-5} s.

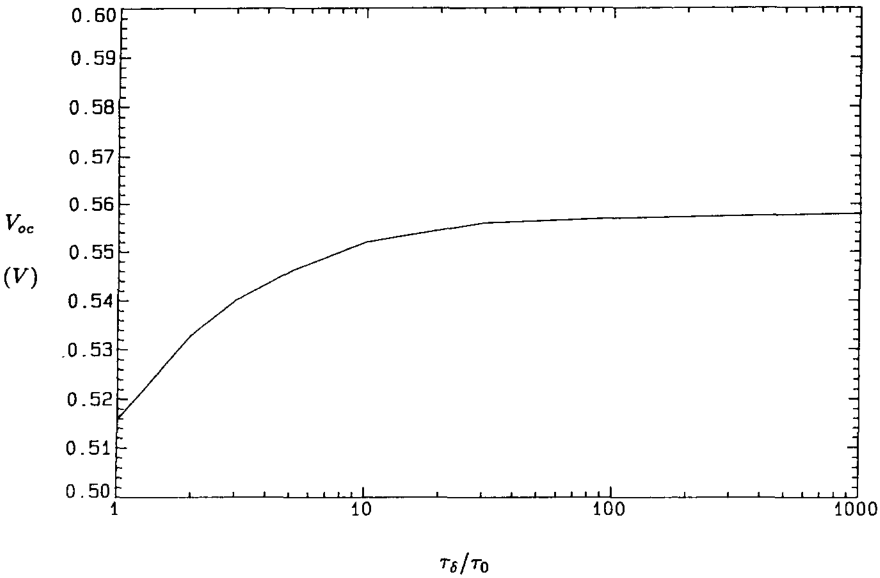

Fig. 5. V_{oc}-improvement as a function of the ratio of lifetimes within the inverse-delta-doped layer to that of the remainder of the symmetrical device of Fig. 2. Here a layer width of 5 nm is assumed.

For the full benefit of the V_{oc}-improvement, it suffices to have the recombination center density reduced by two orders of magnitude, with most of the shift already achieved when N_r is reduced by a factor of 10 (See Fig. 5).

The positioning of the delta-doped or the inverse-delta-doped layer is critical to maximize the influence on performance. This is shown in Fig. 6 for V_{oc} and FF with an inserted layer of 5 nm width and a lifetime that is increased (inverse

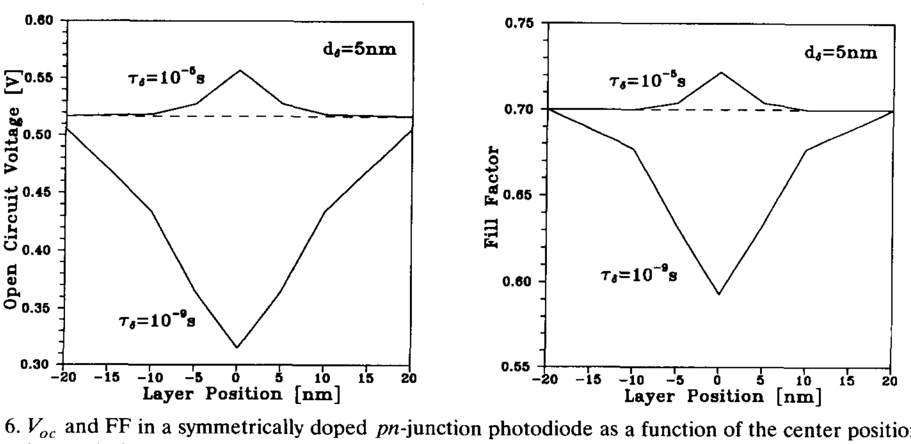

Fig. 6. V_{oc} and FF in a symmetrically doped *pn*-junction photodiode as a function of the center position of an inserted sheet of 5 nm thickness with increased (upper curves) or decreased (lower curves) minority carrier lifetime. Bulk carrier lifetime is 10^{-7} s.

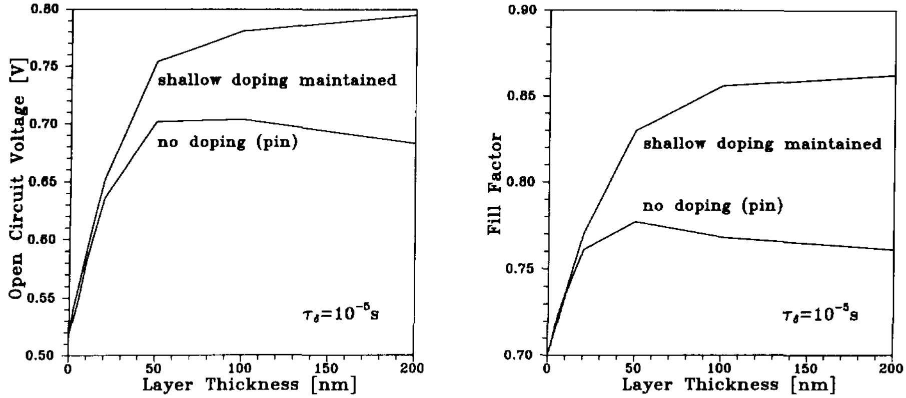

Fig. 7. V_{oc} and FF changes as a function of the width of an inserted inverse-delta-doped layer (upper curves) and of an additional *i*-layer (lower curves). Both layers are centered at the metallurgical interface of a symmetrically doped GaAs *pn*-junction with the same device parameters as used for the computation in the previous figures.

delta-doped) or decreased (delta-doped) by a factor 100 or 0.01, respectively. Positioning the inverse-delta-doped layer only 5 nm from the position where $n \simeq p$, almost completely eliminates the beneficial effect of such a layer.

3. Inverse-delta-doped or i-layer

When, in addition to depriving the thin inserted sheet of recombination centers, as described above for inverse-delta-doping, one also eliminates donors *and* acceptors within this layer, one obtains, in an ideal case, an i-layer.

The insertion of such an i-layer, instead of an inverse-delta-doped layer has a similar effect in improving the performance of solar cells, as long as this i-layer is very thin (10–15 nm). With increasing i-layer thickness, however, the performance improvement stops and then reverts into a performance degradation as is shown in Fig. 7 for V_{oc} and FF. The computation was done for the same example of a symmetrically doped GaAs photo diode as shown for the previous figures.

4. Performance dependence on the optical generation rate

All of the above reported results are obtained at a low optical generation rate of 10^{16} cm^{-3} s^{-1}. Here, the effects of improving the j–V characteristics are relatively large. With increasing optical generation, we still observe a substantial degradation of the device performance with the insertion of a delta-doped layer with increased recombination, however, an inverse-delta-doped layer no longer provides a significant improvement.

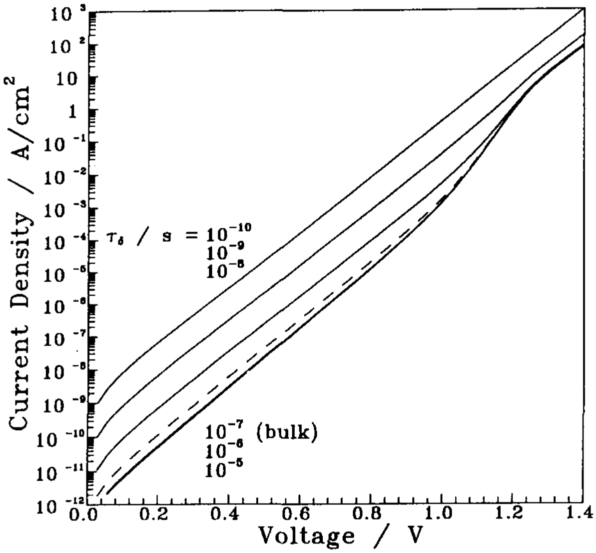

Fig. 8. Dark j–V characteristics of the symmetrically doped GaAs *pn*-junction device as shown in the previous figures, however, with a 5 nm thick interlayer that is centered at the metallurgical interface an contains various densities of recombination centers resulting in minority carrier lifetimes listed as family parameters. The remainder of the device has a minority carrier lifetime of 10^{-7} s. The dashed curve is computed without an inserted sheet.

This can best be seen from the dark j–V characteristics in forward bias, that are shown in Fig. 8 for a number of devices that contain a thin sheet of 5 nm thickness centered at the junction interface of a symmetrically doped GaAs cell. The minority carrier lifetime in these sheets is the family parameter.

The open-circuit voltage can be obtained from this figure by using the superposition principle, i.e., by subtracting from the shown dark current the reverse saturation current ($\simeq$ the short-circuit current, j_{sc}). The open-circuit voltage can, therefore, be obtained from the intersect of this set of curves with a horizontal line at j_{sc}. With such current densities typically at 20–40 mA/cm^2, we are in a range in which the dark j–V characteristic of a high-efficiency cell is steeper, and has a diode quality factor that is near 1, thereby compressing the branches of the shown family while only such devices with substantially enhanced junction recombination still show a marked performance degradation.

5. Donor–acceptor pair recombination in real solar cells

The computation for high-efficient GaAs- and Si-solar cells with the best currently available parameters show a reasonable fit to the observed short-circuit current, but still a substantial lag for V_{oc} and FF between the theoretical values and the best experimental observation. For instance, for GaAs, the best observed

V_{oc} lies below 1.02 V, while from the computation of a device without additional junction recombination one expects $V_{oc} \simeq 1.12$ V.

This discrepancy is too large to be accounted for by cell imperfections and is unlikely the result of neglections in the governing set of equations.

This seems to indicate that sufficient recombination centers always remain close to the cross-over point of $n(x)$ and $p(x)$. Close donor–acceptor pairs [6] could act as effective recombination centers. Such pairs are plentiful at and near the metallurgical interface. Their density depends on the actual process of the junction formation.

Since donors and acceptors, when ionized, are Coulomb-attractive to each other, they tend to form close pairs when the junction is produced via diffusion of the dominant dopant (usually the donor in a p-type base). This results in a layer of enhanced recombination via donor–acceptor pairs throughout the heavier doped n^+-layer. The most effective part for degrading V_{oc}, however, is close to the interface, and extending into the lower doped region. Presently it is not known how large a density of these donor–acceptor pairs extends into the region where $n \simeq p$, i.e., where the performance of the device is most sensitive to recombination centers. It is, however, probable that compensation extends into the lower doped region and creates a thin sheet that is partially compensated, thereby moving the performance-sensitive region closer to the metallurgical interface where close donor–acceptor pairs are plentiful.

When the junction is produced by epitaxy, one would expect a lower density of such pairs to form. This may be a reason why these devices show indeed a somewhat higher V_{oc}. On the other hand, during the growth there is substantial mobility along the surface as each layer is completed, and again this is conducive to close pair formation.

It is, therefore, suggestive to devoid a thin inner layer of the inverse-delta-doped sheet from shallow dopants, thereby physically separating donors from acceptors. When done by MBE, this could effectively eliminate close pair formation and rely on recombination exclusively by distant pairs (and other deep-level impurities that have escaped purification). Such distant pairs may still have substantial recombination probabilities, however, they no longer accumulate, but are statistically distributed when their inter-ion distance exceeds a value in which they can form bond pair centers. Consequently, their concentration will be lower.

6. Summary

High-efficient solar cells are believed to have a degraded V_{oc} and FF due to an increased density of recombination centers, probably because of bond close donor–acceptor pairs in the highly doped (n^+) region, and extending into the region where $n \simeq p$.

Since performance degradation is most effective where $n \simeq p$, it may be sufficient to concentrate efforts of reducing such close pairs near this interface. This may be achieved by the introduction of an inverse-delta-doped sheet that is deprived of deep-level centers, and contains a thin innerlayer that is also deprived of shallow donors and acceptors. The position of this sheet is critical for optimizing its beneficial effect.

Acknowledgement

This work is dedicated to Bernhard Seraphin at the occasion of his 70's birthday.

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