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# Modelling of semi-conductor diodes made of high defect concentration, irradiated, high resistivity and semi-insulating material: the current–voltage characteristics

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**Abstract**

Diodes containing a high concentration of generation–recombination centres can behave in a way, which is not predicted by standard diode theory. Full one-dimensional modelling is reported of the current through a long PIN semi-conductor diode with different concentrations of shallow donors and acceptors, deep donors and acceptors, and generation–recombination centres. From these results we present a physical understanding of the processes involved. The effect on the observed properties for short diodes is also described. An approximate analytical approach is given for a diode with a high defect concentration to complement the standard equations for a diode with a low defect concentration. The results should aid the understanding of the properties of experimental diodes, give an indication of the types of traps in the material and also suggest how their properties may be modified by additional doping. There are specific applications of these results to radiation damaged devices, lifetime killed diodes and devices made from high resistance and semi-insulating materials.



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## 1. Introduction

Many poorly conducting semi-conducting and semi-insulating electronic materials show unusual electrical properties such as non-Ohmic behaviour. These experimental findings are often tacitly ascribed to their highly impure state with many defects and impurities, but not analysed in detail.

The materials and structures to which this study can apply are very extensive: intrinsic, high-resistivity, highly irradiated or lifetime killed semi-conductors and semi-insulators formed into junction or Schottky diodes. To study such samples in detail experimentally, to find out their material properties and hence the origin of the observed effects is usually very difficult. They are often highly impure and defected so that there is

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an array of energy levels within the forbidden band. The amounts and types of these are unknown and often too large to be determined readily. Some analytical techniques may not correctly measure the concentrations because of the method used and the assumptions in the analysis are usually those appropriate for normal, lifetime, nearly pure semi-conductors. This will become apparent later as the physics of relaxation diodes is described. Fortunately, it can be seen in experiments, and confirmed by the present modelling, that many of the properties that are observed are generic and do not depend very much on the details. In particular, the details of the contacts, P–N junction or Schottky, abrupt or slightly graded, are not very important to the basic effects seen. Similarly, it is the dominance of a particular type of defect, shallow or deep, donor or acceptor that is the main criterion rather than their specific densities and energies. The necessary conditions are that the material has a high resistivity, that is it is a nearly intrinsic or compensated semi-conductor or semi-insulator, and that it has a very high density of generation–recombination (g–r) centres. That is, it is a relaxation rather than a lifetime semi-conductor. This will be described later.

Most previous calculations have been carried out mainly as a demonstration of the relaxation theory [1], others have been done to show that experimental observations are consistent with a specific model [2,3]. The present work is designed as a practical and helpful analysis to enable the experimenter to understand the internal state of his sample and what its likely impurity content is. Here we describe the main features, which are observed experimentally, model them using a typical diode structure as an example, explain the physical processes occurring and discuss the implications and applications. The aim is to explain the physical reasons underlying the experimental results and the effects of different types of defects. By making this range of generic calculations with different parameters we have established that the results obtained are robust and insensitive to the details of the sample such as the type and magnitude of the trap energy levels so that general categories such as deep or less-deep levels can be considered. In each case the change with the g–r centre concentration is given. The variation with trap concentration or cross-section can be deduced from the analytical calculation. This should enable some general idea to be obtained about the dominant defect content of any specific device and how its properties may perhaps be modified by additional doping. However, any particular study may require a detailed analysis of the type presented here.

A considerable number of experimental results have been reported of electrical measurements, current–voltage and capacitance–voltage, on samples which undoubtedly fulfil the relaxation criterion but only a few give full results, forward and reverse bias on a logarithmic scale so that full comparison with this modelling can be made [4–10]. The main electrical features which are illustrative of a diode behaving in this way, and needing this interpretation, are: an Ohmic resistance up to about 1 V with a slowly increasing (sub-Ohmic) current in one direction and more rapidly increasing in the other for an asymmetric diode but only slowly increasing for a diode with both contacts blocking. The resistivity demonstrated by the Ohmic region is the maximum resistivity, approximately that of the intrinsic material. To see understandable effects the sample must be asymmetric, $P^+$–$N^-$–$N^+$, with one junction and an Ohmic contact, since blocking contacts in series opposition largely reveal only the reverse bias characteristic. A log−log plot is best to expose the general behaviour.

The many other results which have been reported are compatible with these results but do not have the necessary completeness to enable an interpretation by a relaxation analysis. This is because the very basic properties: asymmetric conduction and a general decrease in the capacitance with increasing reverse voltage are broadly similar to those of normal diodes, although the details are very different. Such near-Ohmic results on a high-resistance sample, such as a semi-insulator, are often interpreted, with relief usually, as a good Ohmic contact. Thus exact results on structures made of these materials are rarely interpreted or displayed in a helpful way especially since the contacts are often identical and hence the characteristic will be dominated by the blocking contact. However, the internal behaviour is very different from that of a sample with true Ohmic contacts as can be seen from the details of the current–voltage characteristics. The capacitance is found to be broadly similar to that of a normal depleting diode in reverse bias but in forward bias its value is low, rather than increasing and it can become negative rapidly [10]. The forward bias capacitance may be difficult to observe since there is a large parallel conductance.

There are also other diode conduction effects observed in such devices, such as double injection [11] and space-charge-limited conduction [12] but these give different and recognisable current–voltage characteristics.

## 2. Modelling and experiments

The modelling was carried out using the package KURATA [13]. The structure is divided into $N$ points along the $x$-axis. A higher density of points was used near the metallurgical junctions. The programme uses an explicit integration method to solve the one-dimensional Poisson, current density and continuity equations for electrons and holes. The variables computed are the electron density, $n$, the hole density, $p$, and the potential, $V$, at each mesh point of the structure.

The initial values of $n$ and $p$ are simply the corresponding doping densities, that is in the $p$-region $p = N_A$ and $n = n_i^2/N_A$ while in the $n$-regions $n = N_D$ and $p = n_i^2/N_D$. Here $N_A$ and $N_D$ are the local acceptor and donor densities. The boundary conditions are: at the far end of the $P^+$ contact: $p = N_A$, $n = n_i^2/N_A$ and $V = 0$ (the reference voltage). At the far end of the $N^+$ contact: $n = N_D$, $p = n_i^2/N_D$ and $V$ = the applied voltage.

The other variables can be computed once $n$, $p$ and $V$ are known. For example the electric field, the Fermi level, the space charge density, the capacitance, etc. The current is calculated from the current density equation.

### 2.1. The sample

The analysis was carried out for a silicon $P^+N^-N^+$ structure with $4\times10^{12}\,\mathrm{cm}^{-3}$ shallow donors ($N^-$). The contacts are $P^+$ ($N_A = 1\times10^{15}\,\mathrm{cm}^{-3}$) between 0 and 25 μm and $N^+$ ($N_D = 1\times10^{15}\,\mathrm{cm}^{-3}$) between 325 and 350 μm. The area is 0.01 cm$^2$ and the temperature 300 K We assume sharp metallurgical junctions although we have confirmed that the more realistic graded junctions make little difference since the junction region itself is mainly depleted. That is, the details of the contact do not matter much. A deep contact region has been assumed to ensure that there is insignificant depletion at $x = 0$, 350 μm.

The intrinsic carrier concentration at room temperature, $n_i$, is $1.45\times10^{10}\,\mathrm{cm}^{-3}$ and is hence much less than the donor density. The dielectric relaxation time, $\tau_D$, at room temperature is about $10^{-9}$ s so the relaxation criterion is reached for a value of the g–r centre density of $N_{GR} \sim 10^{16}-10^{17}\,\mathrm{cm}^{-3}$ using $\tau^{-1} = \sigma v_{th} N_{GR}$, where $v_{th}$ is the thermal carrier velocity, and a typical value of $10^{-14}\,\mathrm{cm}^{-2}$ is used for the cross-section, $\sigma$ [14].

We consider the cases with different added traps as the density of generation–recombination (g–r) centres at mid-gap is increased from $10^7$ to $10^{18}\,\mathrm{cm}^{-3}$. In this model, we consider these g–r centres to have no net charge. This gives a very simple separation between the effect of traps, which are charged when unoccupied, and g–r centres. Not much is known about these centres. In the calculations we have simulated a charge on the g–r centres by adding traps near mid-gap and there have been no significant differences in the results from those described. This will be seen by the results presented which show little change in the average space charge when deep traps are added. Experimental results on irradiated silicon seem to suggest that they have no net charge since no space charge, measured by the average space charge $N_{eff}$ from the depletion voltage of the C–V plot to full depletion, can be ascribed to these centres. Typical values of $10^{13}$–$10^{14}\,\mathrm{cm}^{-3}$ are measured when the experimental $I$–$V$ plots, compared with the modelled plots, suggest concentrations of g–r centres of $10^{17}\,\mathrm{cm}^{-3}$ [7]. However, in silicon this may have to be reassessed [15]. The calculations are also made for the sample with the addition of deep donors (DD) at $E_T = E_V + 0.4\,\mathrm{eV}$ and/or deep acceptors (DA) at

$E_T = E_C - 0.4\,\text{eV}$. These traps interact most with their own band. The concentrations are $4\times10^{14}\,\text{cm}^{-3}$, which is less than the contact concentration. The energy gap in silicon is 1.12 eV. Since the traps only contribute to the space charge in this static calculation the cross-section is not important provided the small retrapping of the generated free carriers is neglected. The density and energy of these deep levels has been found to not change the basic results. We will not consider the case with both DD and DA in detail since the interpretation follows from the separate analyses. We have also considered the case where 'less deep' donors (LDD) or acceptors (LDA) are added with energies $E_T = E_V + 0.6\,\text{eV}$ and $E_T = E_C - 0.6\,\text{eV}$. In this nomenclature shallow donors have energies less than the thermal energy and are hence normally ionised. Deep levels are on the far side of mid-gap compared with the shallow levels and 'less deep' levels are on the same side of mid-gap as the shallow levels but have an energy much greater than the thermal energy.

The physical interpretation given here is based on the understanding given by the calculated spatial variation of the various quantities such as; free electron and hole densities, space charge density, electric field, generation/recombination rate although these are not shown here.

For small bias (forward or reverse) the characteristics are not dependent on the far $N^-$–$N^+$ contact and hence represent the semi-infinite, long diode, case. This has been checked by modelling a single $P^+$–$N^-$ junction. However, this 'far contact' does affect the *I–V* characteristics in general, and for short diodes especially and this is discussed briefly. The far contact has a major effect on other properties such as the electric field profile and the C–V characteristics and we will report these later.

## 3. The P–N diode

We will now review the behaviour of a conventional, lifetime, diode so that there is a good basis of comparison and the differences are drawn out. The change in the characteristics with increasing density of g–r centres can then be considered as a description of the characteristics of a diode as it is made more impure. Consider the semi-infinite case with few g–r centres. This is the 'lifetime' case as appears in standard texts [14]. The current is due to the diffusion of carriers to the junction and is given by

$$I = I_{01}\{\exp(eV/kT) - 1\} \tag{1}$$

which is exponential in forward bias and saturates in reverse bias. For forward bias, if $eV > kT$, we can approximate this by

$$I = I_{01}\exp(eV/kT). \tag{2}$$

The prefactor controls the reverse saturation current and the zero-voltage impedance and is [14]

$$I_{01} = Aen_i^2(D_p/\tau_p)^{1/2}/n_{n0} \tag{3}$$

where $n_i$ is the intrinsic carrier density, $D_p$ and $\tau_p$ are the hole diffusion constant and lifetime and $n_{n0}$ is the equilibrium electron density on the *N*-side of the junction and *A* is the junction area. The zero-voltage conductance is

$$Ae^2n_i^2(D_p/\tau_p)^{1/2}/kTn_{n0} \tag{4}$$

which varies as $N_{GR}^{1/2}$ if $\tau \sim N_{GR}^{-1}$ and has a temperature dependence due mainly to the activation energy, $E_g$, of $n_i^2$.

In real diodes there are g–r centres which act as very efficient electron–hole pair generators or recombiners. As discussed earlier we assume that they are electrically neutral. For this high efficiency the Fermi energy must be either at this mid-gap energy or, away from equilibrium in the space charge region, the quasi-Fermi levels must be separated across the mid-gap energy. Then there is a generation or recombination current with a size dependent on the g–r centre efficiency and density and the volume, or width, of the active area, such as the depletion region [14], and given by

$$I = I_{02}\{\exp(eV/2kT) - 1\} \tag{5}$$

which is exponential in forward bias. The factor 2 in the exponent derives from the two-step g–r process. For forward bias, if $eV > 2kT$, we can approximate this by

$$I = I_{02}\exp(eV/2kT). \tag{6}$$

We can approximate the prefactor

$$I_{02} = CAWn_iN_{GR} \tag{7}$$

where $C$ is a constant depending on the efficiency of the centres, the sign of the bias (i.e., generation or recombination) and $W$ the depletion width. This produces the characteristic $V^{1/2}$ variation in reverse bias corresponding to the voltage dependence of the active depletion width [14].

The zero-voltage conductance is then

$$CAW_0n_iN_{GR}e/2kT \tag{8}$$

which varies as $N_{GR}$, and has an activation energy mainly due to $n_i$, of $E_g/2$. In this case, $W_0$ is the depletion width of the built-in voltage (which has been neglected in the above).

$$V_{bi} = eW_0^2n_D/2\varepsilon\varepsilon_0 \tag{9}$$

and $V_{bi} \sim E_g/2e$ for the highly asymmetric junction considered here and $n_D$ is the space charge density equal to the net ionised donor, or acceptor, density. In forward bias the voltage variation of $W$ is small.

In a real diode both the diffusion current and the generation (reverse) or recombination (forward) currents exist together. This is very noticeable in the log-linear presentation of the forward current–voltage characteristic, which has a slope $e/kT$ at high voltages and the lower slope $e/2kT$ at lower voltages. Since very low currents need to be measured, and the transition between the slopes appears slow, the curve measured over a limited voltage range is often approximated to

$$I = I_0\{\exp(eV/\eta kT) - 1\} \tag{10}$$

with $\eta$ between 1 and 2.

There is another effect that can appear in the current–voltage characteristics of a real diode at high currents. This is seen especially in a diode with special requirements such as the transparency of one contact in a solar cell or photodiode, or in diodes of special materials such as high-resistance semi-conductors. This is the effect of the resistance, $R_s$, of the contact and any neutral semi-conductor in series with the actual junction. The voltage dropped across this circuit element reduces the part of the terminal voltage, $V$, appearing across the junction itself. Thus, the total current given by the sum of the diffusion and g–r currents of (1) and (6) becomes

$$I = I_{01}\{\exp(e(V - IR_s)/kT) - 1\} + I_{02}\{\exp(e(V - IR_s)/2kT) - 1\}. \tag{11}$$

In reverse bias the current is small and the presence of $R_s$ produces no change. Similarly at low and medium forward currents. However, at high forward current the characteristic becomes Ohmic with a resistance $R_s$.

These standard results would suggest that as the density of g–r centres is increased, more electron–hole pairs are thermally generated and the current in forward and reverse bias will increase. However, this does not continue to infinitely large currents because the electrical properties of the material change considerably and it becomes a 'relaxation' semi-conductor rather than the conventional 'lifetime' semi-conductor. It is this transition that interests us here.

The conventional 'lifetime' material has $\tau_D \ll \tau_0$. A 'relaxation' material has $\tau_D \gg \tau_0$. Here $\tau_D = \rho\varepsilon\varepsilon_0$ ($\rho$ is the resistivity) is the dielectric relaxation time which is the time in which a space charge is neutralised by the flow of the free carriers drawn in by the charge but slowed down by the resistance. It is the bulk equivalent of an RC time constant. The minority carrier recombination lifetime, $\tau_0$, is the time constant for recombination of non-equilibrium electron–hole pairs or excess minority carriers. It is also the time to generate electron–hole pairs to reach equilibrium. In lifetime material charge flows inwards rapidly to cancel any non-equilibrium space charge and local charge neutrality is an equilibrium requirement which is usually used as one of the basic equations. In relaxation material there is a local generation or recombination of carriers. A material will become relaxation-like if it has a high resistivity (near intrinsic or compensated) and a large density of defect generation–recombination (g–r) electronic levels near the middle of the energy gap which can readily interact alternately with electrons and holes. Such traps can be produced by radiation damage (as in irradiated silicon devices) or some dopant impurities such as those that create semi-insulating GaAs or silicon which has had the carrier lifetime 'killed' by the addition of gold.

Consider a depletion region in a relaxation-like semi-conductor. Electron–hole pairs are generated (or recombine) readily 'on demand' if the continuity or electrostatic equations demand more carriers. For a steady state in the charge distribution the currents flowing on each side of the generation point are continuous so that $n_0\mu_n = p_0\mu_p$ and with $n_0p_0 = n_i^2$ we get $n_0 = p_0(\mu_p/\mu_n) = n_i(\mu_p/\mu_n)^{1/2}$ and in this steady state these equilibrium carrier densities, $n_0$ and $p_0$, are independent of the specific material, contacts or traps. Here $n_i$ is the intrinsic carrier concentration and $\mu_{n,}$ $\mu_p$ are the electron and hole mobilities. The resistivity is then at its maximum value given by

$$\rho^{-1}\max = (2en_i(\mu_n\mu_p)^{1/2}) \tag{12}$$

which has a value $\sim(8\times 108\,\Omega\,\text{cm})^{-1}$ at room temperature for GaAs and $(3\times 10^5\,\Omega\,\text{cm})^{-1}$ for silicon. Note that this has similar properties to the intrinsic material with $n = p = n_i$ and a resistivity given by $\rho^{-1} = (2en_i(\mu_n + \mu_p)/2)$. This is one coincidence that has hidden the true behaviour of such materials. The physics of these two materials is very different. Under bias the material is not in equilibrium so there must be separate quasi-Fermi levels for electrons and holes. In a normal junction made of lifetime material the Fermi level is uniform throughout the junction under zero bias but the electron and hole quasi-Fermi levels are split under bias. In reverse bias they are above and below the g–r centres in some part of the depleted junction so that electrons and holes are alternately emitted. A significant feature of a highly relaxation-like material is that the two quasi-Fermi levels merge near mid-gap. For an ideal material with an infinite density of active g–r centres the generation rate for any centre tends to zero and the Shockley–Read equation then gives $n_0p_0 = n_i^2$. This is the justification for the use of this expression in the analysis above, not the normal reason that the material is in equilibrium.

Thus, for a material with suitable properties, made into a junction, there will be a length with active g–r centres, which is acting as a relaxation material and has this maximum resistivity. In a given piece of material not all of it will be acting as a relaxation semi-conductor since for this the g–r centres must be active, which requires that the quasi Fermi levels are near mid-gap. Thus, it is not easy to make simple approximations to describe the behaviour such as is done for diodes made of the conventional lifetime material. An approximate analytical model will be given later.

The results of the modelling are shown in Figs. 1(a)–(e) for the cases of no deep levels, deep donors only, deep acceptors only, less deep donors only and less deep acceptors only. The results are presented on log–log scales with forward and reverse curves superimposed. In each case the density of the g–r centres is increased in decades from $10^7$ to $10^{18}\,\text{cm}^{-3}$. The apparent noise is due to the calculation procedure. Fig. 2 shows experimental results on irradiated silicon diodes, which have been presented before [4] but are shown here for completeness. Other results have been presented before on diodes made from semi-insulating GaAs both irradiated and non-irradiated [9,16]. These plots show the basic features produced by the simulations such as the low-field Ohmic region, the increase in the low-field conductance with irradiation and the limiting maximum resistivity which extends over a larger voltage range with increasing fluence.

### 3.1. No deep traps

Fig. 1(a) shows the curves increase monotonically with increasing $N_{GR}$. There is less sensitivity to the g–r centre density at low and high values of the parameter. The significant Ohmic lines of $R_s$, upper line and $R_{max}$, bold line, are drawn for comparison. These are calculated for all the material between the highly doped contacts.

For a very low density of g–r centres the forward and reverse currents follow the ideal diffusion current. The reverse diffusion current saturates. The curves separate at about $V = kT/e$ (26 MeV). This is derived from the energy balance in (1) and (5) but also represents the voltage below, which the built-in voltage and its depletion region dominates.

Above $N_{GR} \sim 10^9\,\text{cm}^{-3}$ in reverse bias we see the generation current from within the depletion region which grows as $V^{1/2}$. The curves move up as the g–r density increases roughly proportional to $N_{GR}$ as given by Eqs. (6), (7) and (8). At this

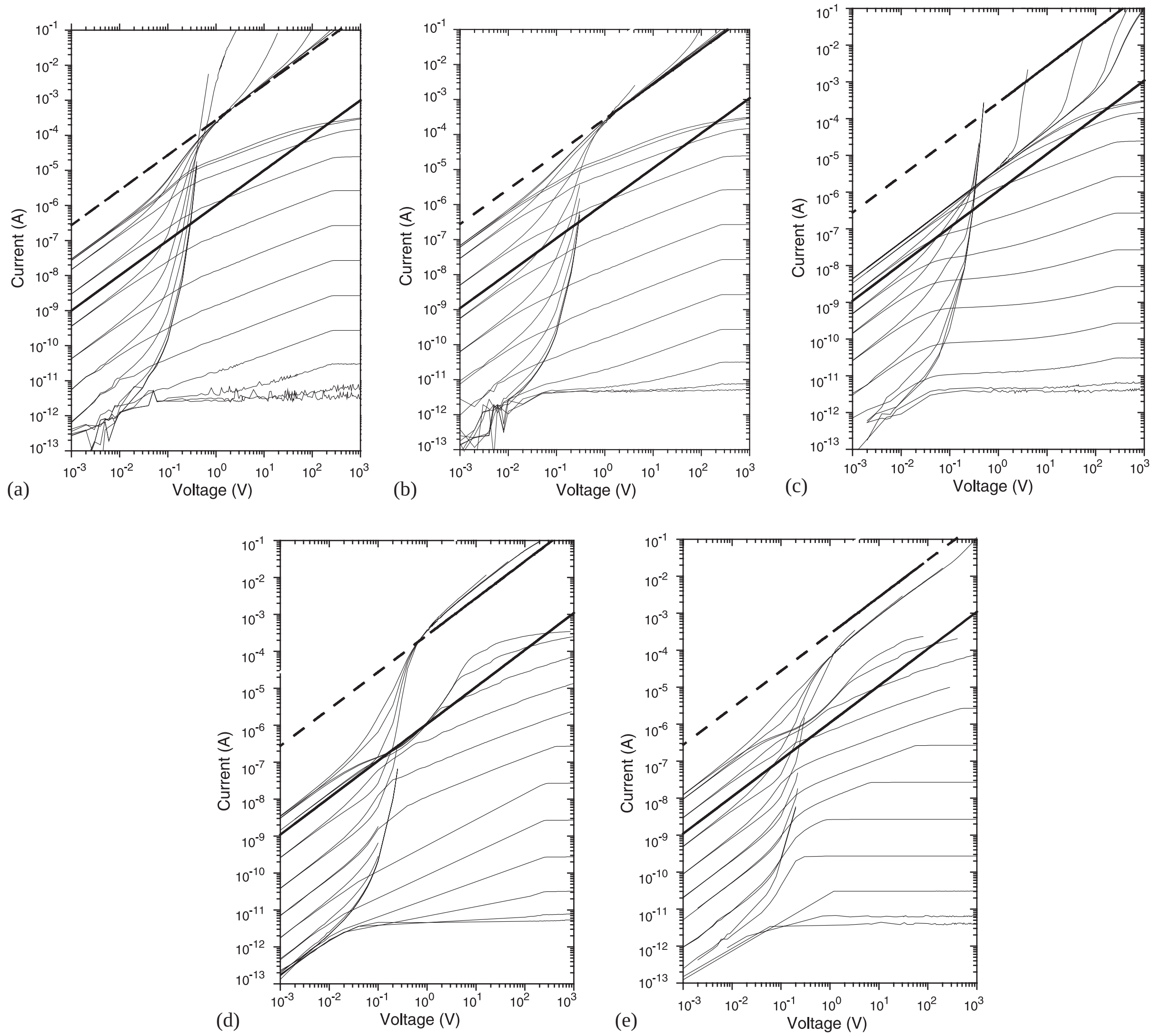


Fig. 1. Modelling results for the current–voltage curves of a semi-conductor $P^+N^-N^+$ diode with the properties given in the text and with an increasing density of g–r centres, in decade steps from $10^7$ to $10^{18}\,\text{cm}^{-3}$ as the curves move progressively upward. The area is $0.01\,\text{cm}^2$. The bold Ohmic line is for the whole diode material at the maximum resistivity and the upper line is for the material at the neutral resistivity. Graph (a) is with no deep traps, the others are for a concentration of $4\times10^{14}\,\text{cm}^{-3}$ of (b) deep donors, (c) deep acceptors, (d) less deep donors and (e) less deep acceptors.

shallow donor doping density the sample is fully depleted at about 270 V. The zero-voltage conductance also scales as $N_{GR}$ as given by (8).

At high values of $N_{GR}$ the two Ohmic lines provide a framework for the characteristics. The forward bias curve is often limited by the series resistance $R_s$, as in Eq. (11). At slightly lower values of $N_{GR}$ there is some excess breakdown current and we will discuss this later. Near zero volts the resistance is dominated by the maximum resistivity relaxation material within the depletion region of the built-in voltage. The reverse characteristic tends to the limit of the $R_{max}$ value when there is full depletion, the current saturates, and

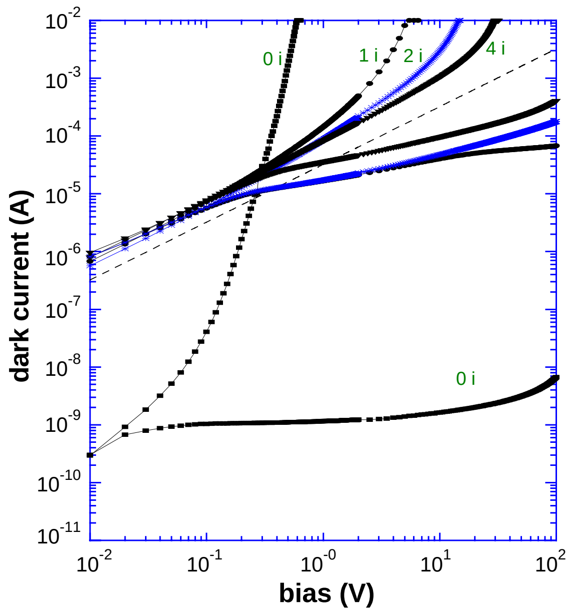


Fig. 2. Experimental $I-V$ curves of silicon $P^+N^-N^+$ diodes irradiated at neutron fluences of 0 (0i), 0.34 (1i), 0.83 (2i) and 2.50 (4i) $\times$ $10^{14}\,\text{ncm}^{-2}$ to show that the curves get closer to the maximum resistance curve, shown dashed, as the damage increases [1].

the entire sample is relaxation-like. At lower voltages the device is a series combination of the junction depletion layer, the maximum resistance section and the part of the series resistance that is undepleted. This will be developed in the analysis section later. These three Ohmic sections provide the limits. The existence of Ohmic characteristics for this diode structure is one reason why there has been little appreciation that the structure is really a diode. It is possible that incorrect assumptions have been made about the type of contacts, which have been made to such materials and the internal structure, especially the position of the quasi-Fermi levels.

The reason for the apparent breakdown at forward voltages for high g–r centre concentrations can be deduced from the variation of the carrier concentrations at different voltages. The breakdown occurs when there are electrons and holes in excess of the equilibrium densities in the series resistance material due to high injection from the contacts and the diffusion length is longer than the diode length.

### 3.2. With deep donors

The main differences from the first case can be seen in the Fig. 1(b).

(a) All the curves dominated by the g–r currents at medium $N_{GR}$ are very similar to the case with no deep traps. The deep donors have no effect on the generation/recombination rate since they are far from mid-gap and are hence not active as g–r centres. Also, they do not contribute to the depletion region space charge since for relaxation-like materials the common quasi-Fermi level is near the mid-gap so that these deep donors are electrically neutral. The reverse voltage where the current saturates remains the same.
(b) The apparent breakdown is reduced since a higher voltage is required for the density of the injected electrons and holes to exceed the density of the shallow plus the ionised deep donors near the contact.

### 3.3. With deep acceptors

Where the Fermi energy is suitably located, the deep acceptors compensate the shallow donors to reduce the free electron density. They are also negative when they have absorbed a free electron so that they also compensate the space charge. This compensation helps the g–r centres to reach the relaxation criterion.

(a) The diffusion current and zero-voltage conductance at very low $N_{GR}$ are the same.
(b) The g–r currents at low voltage and medium $N_{GR}$ have increased because the built-in voltage depletion width is larger.
(c) At low and medium $N_{GR}$ the reverse bias curves move up and appear saturated as for a diffusion current because the whole device is fully depleted at a very low voltage. The saturated value of the current is the same as the current at 270 V, the full depletion voltage for the no deep levels case.
(d) The Ohmic limiting curve at very high $N_{GR}$ is now very close to the $R_{max}$ limit since the neutral material is compensated to be nearly intrinsic. The series resistance line shown as

the value for the material without deep levels, for reference, but for this case $R_s$ is at the intrinsic conductance which should be a little higher than the maximum resistance line as seen.

(e) The breakdown point is lower since a smaller voltage is now required for the injected electrons and holes to exceed the reduced compensated shallow donors. However, the current increases rapidly.

(f) At large $N_{GR}$, the divergence voltage between the forward and reverse curves moves to a higher value. This is because the reverse current at the full depletion voltage is always the same size (for a given $N_{GR}$) so that, since the lines are all getting closer together the break must occur at a higher voltage.

### 3.4. With both deep donors and deep acceptors

We do not present this data since the results can be deduced from the combination of the effects seen separately above. From the discussion it can be seen that the exact position and concentrations of the deep levels is not very important for the types of effect seen.

### 3.5. With added less-deep donors or acceptors

We have included in the model calculations the cases where less deep acceptors or donors are added. These are deep levels but on the 'other side' of mid-gap. That is they are on the same side as for shallow donors or acceptors, but deep enough that they are not normally fully thermally ionised. These could be significant to some properties of relaxation diodes since they will change their charge state when the quasi-Fermi level moves to mid-gap as the material changes from lifetime to relaxation-like.

The presence of less deep donors is shown in Fig. 1(d). The main effect is to make the material far less relaxation-like as can be seen by the divergence of the forward and backward characteristics remaining at about $kT/e$ for large $N_{GR}$. There is a very large increase in the voltage for full depletion as $N_{GR}$ increases because of the increase in ionised donors with voltage as the quasi-Fermi energy moves towards mid-gap. The low-voltage conductance is lower because the zero bias depletion width is less, as in Eq. (9). The forward bias curves tend to the value of the neutral material with a doping of $4\times10^{12}$ as shown by the dashed line, $R_s$. It goes above the line because some of the less deep donors are ionised.

The less deep acceptors shown in Fig. 1(e) again suppress the progress to the relaxation-like state and the forward bias state are similar to the neutral semi-conductor. There is compensation of the shallow donors as for the deep donors. At low $N_{GR}$ this reduces the depletion voltage but as the Fermi energy moves towards mid-gap at larger $N_{GR}$ the less deep acceptors become ionised to increase the space charge and the depletion voltage. There is type inversion. Thus, in general the less deep traps act in a similar way to shallow traps and reduce the progress to the relaxation state by moving the Fermi level away from mid-gap.

There is an apparent 'cross-over' in the forward and reverse characteristics. This is simply because of the detailed shapes of the curves and has no practical effect. In large forward bias and $N_{GR}$ the characteristics are dominated by $R_s$ as in (11). The actual value is not exactly equal to the value predicted by the shallow donor concentration because some of the less deep donors and acceptors are ionised by the movement of the quasi-Fermi energy towards mid-gap. Also, the breakdown is suppressed for the same reason.

For the less deep donors the zero voltage conductance is lower because of the decrease in the width $W_0$ due to the increase in the space charge and a reverse effect occurs with the less deep acceptors.

For the less deep acceptors in the depletion region there is over-compensation to give a space charge of the opposite sign. $V_{dep}$ goes to zero and then becomes very large as $N_{GR}$ increases. Thus, 'type inversion' is seen even though less deep traps, rather than shallow acceptors are involved.

## 4. Analytic I–V characteristics

For completeness we include here an analytical treatment of the $I$–$V$ characteristics of diodes made from near relaxation material. In such a complex system this involves fairly large assumptions and hence approximations. However, this approach may be easier to use than the full modelling, when the sample has a large value of $N_{\mathrm{GR}}$.

The first case is the case with zero space charge so that the whole diode is a region of Ohmic relaxation material with Ohmic characteristics. From before the resistance is

$$1/G_0 = R_0 = \rho_{\max} d/A \tag{13}$$

where $d$ is the distance between the contacts and $A$ is the diode area. The blocking properties of the junction have disappeared. Although it is an Ohmic resistance its physics is not the same as a normal resistor.

Now we consider the case of a diode made with near-relaxation material with very small space charge. This corresponds to a low donor/acceptor density and a low deep level density.

### 4.1. Reverse bias

The total voltage drop across the 'depleted' part of the diode consists of three parts:

1. That due to the current through the Ohmic region which is the relaxation-like section of width $W_1(V)$ and maximum resistivity $\rho_{\max}$ to give a resistance $R_0(V) = 1/G_0 = \rho_{\max} W_1(V)/A$. Since $W_1$ is not well defined we will replace the full expression for $R_0(V)$ by the value derived above, $R_0$, equal to that of a diode of maximum resistivity and full depletion ($W_1 = d$). This works quite well since the approximation that the width is the full voltage-independent geometric width and the approximation that the mobility is that of the undamaged material work in opposite directions.
2. Those due to charge dipole layers:

(i) The normal *built-in voltage,* $V_{\mathrm{bi}}$, which is here equal to half the band gap (about 0.5 V for silicon and hence often negligible) which is the band discontinuity. We represent this by a region of free carrier space charge $n_{\mathrm{f}}$ over a distance $W_0$ or a built in charge of $Q_0 = n_{\mathrm{f}} W_0$. There is a corresponding charge within the contact. There are insufficient ionised defects to account for the built-in voltage and the fact that the material is relaxation-like force a rapid change in the position of the Fermi level at the contact.

(ii) The space charge in the depletion width (and the corresponding charge in the contact). The length $W(V) > W_1(V)$ is the total 'depletion width' where the traps of density $n_{\mathrm{t}}$ are empty. This includes the regions, which are relaxation-like and also where there are separate quasi-Fermi levels. This can be a complex region since the traps may be of different depths and there are also donor/acceptors, which are always ionised.

Thus,

$$V = R_0 I + eW^2 N_{\mathrm{T}}/2\varepsilon\varepsilon_0 + Q_0 W_0/2\varepsilon\varepsilon_0 \tag{14}$$

or

$$V - V_{\mathrm{bi}} = R_0 I + eW^2 N_{\mathrm{T}}/2\varepsilon\varepsilon_0 \tag{15}$$

since, from electrostatics [11] across the depletion region

$$V = eW^2 N_{\mathrm{T}}/2\varepsilon\varepsilon_0 \tag{16}$$

and from Eq. (9)

$$V_{\mathrm{bi}} = eW_0^2 N_{\mathrm{T}}/2\varepsilon\varepsilon_0 = Q_0 W_0/2\varepsilon\varepsilon_0.$$

In a normal diode with g–r centres the quasi-Fermi levels are different for the electrons and holes and there is a generation current proportional to the depletion width and hence varies as $V^{1/2}$. Here we assume that the relaxation width is fairly voltage independent and the generation current is generated over the whole depletion width.

Thus,

$$I = N_{\mathrm{GR}} WA \tag{17}$$

where $N_{\mathrm{GR}}$ is the effective density of g–r centres and includes a factor to account for their efficiency, and

$$V - V_{\mathrm{bi}} = R_0 I + eN_{\mathrm{T}} I^2/2\varepsilon\varepsilon_0 N_{\mathrm{GR}}^2 A^2 \tag{18}$$

or

$$V - V_{\mathrm{bi}} = R_0 I + R_1 I^2. \tag{19}$$

Here $V_{bi}$ is half the band gap and hence is usually negligibly small. The first term on the right-hand side corresponds to the Ohmic relaxation contribution and the second to that of the space charge dipole.

The change from Ohmic to $V^{1/2}$ occurs when these two terms are equal at

$$V_t = V_{bi} + 2R_0 I_t, \quad I_t = R_0/R_1. \tag{20}$$

If we take the case where the irradiation fluence $\Phi$ produces both traps and g–r centres so that

$$N_T = \beta\Phi, \quad N_{GR} = \alpha\Phi \tag{21}$$

then

$$V - V_{bi} = R_0 I + e\beta\Phi I^2/2\varepsilon\varepsilon_0(\alpha\Phi A)^2 \tag{22}$$

so that

$$V_t = V_{bi} + 2R_0 I_t, \quad I_t = 2(\varepsilon\varepsilon_0/e)R_0 A^2(\alpha^2/\beta)\Phi. \tag{23}$$

There are several approximations made here and we know little about their quality but the fit seems to be reasonable. The modelling seems to confirm the quadratic increase in $V_t$ and $I_t$ with $N_{GR}$ as seen in Fig. 1(c). The experimental data are not good since different samples have been used for each fluence value but confirm the linear increase in $V_t$ and $I_t$ with fluence.

### 4.2. Forward bias

Experimentally we find that in forward bias the $I$–$V$ curve fits the exponential function

$$I = G_0 V \exp V/V_0 \tag{24a}$$

or more probably

$$I = G_0 V \exp Vd/E_0. \tag{24b}$$

Here $V_0 = E_0/d$ is a fitting parameter and the particular form preferred depends on the physics involved, a critical voltage or field. This is the fitting function which was used for other relaxation materials years ago [17]. The values of $V_0$ and $E_0$ should be recorded as a simple measure of the degree of relaxation-like-ness. Although these parameters give an indication of the onset of 'breakdown' this is a complex process so that care should be taken in using this fitting parameter as a universal measure of relaxation-likeness. although it may be of value within a single system, or as a very general indicator.

## 5. Summary of modelling results

An impure high-resistivity semi-conductor can be a very difficult substance to understand. The results of this modelling show that the current–voltage curve is characteristic and does not vary in general form over a wide range of trap types and concentrations. The curves are constrained by an Ohmic line representing the resistance of the starting material, without any diode structure. This is revealed at medium and large forward voltages and a high density of generation–recombination centres. At a limiting high reverse voltage, for full depletion, in a diode containing a large concentration of g–r centres, the current is limited by the whole diode being at the maximum resistivity.

The value of the zero-voltage Ohmic resistance is due to the generation current in the built-in voltage depletion region. This is at the maximum resistivity value and provides the limiting conductance of the series elements of the total diode.

The activation energy of the zero-voltage conductance is either $E_g$ or $E_g/2$ as given by Eq. (4) or Eq. (7), or between these values.

The current–voltage plot is valuable to understand the behaviour inside the device. From a comparison of the experimental and modelling plots it is possible to deduce the approximate relative densities of the different types of deep centres. The reverse current becomes saturated for voltages higher than a saturation voltage, $V_{dep}$. The detection of full depletion from the current–voltage characteristics can be valuable to indicate how other measurements, such as the capacitance–voltage should be analysed. In some cases $V_{dep}$ may be determined more clearly from the $I$–$V$ curves than the $C$–$V$ curves, as normally done at present. The $I$–$V$ plots show only saturation when the diode becomes fully depleted whereas the $C$–$V$ characteristics, which show other effects related to the far contact, distort the linear nature of the $C-V^{1/2}$ curve. We hope to show this in a later publication. At full depletion the width $W$ in

Eq. (9) becomes the geometrical length, $d$, and we obtain an equation for $N_{\text{eff}}$, the effective density of space charge within the whole diode.

$$V_{\text{dep}} = ed^2 N_{\text{eff}}/2\varepsilon\varepsilon_0. \tag{25}$$

A $\log I - \log V$ plot is best to reveal the details and needs to be taken from a bias below $kT/e$ to above the voltage for full depletion. From this plot can be seen the closeness of the resistivity to the maximum value, the $V^{1/2}$ region and the current saturation at full depletion in reverse bias and the form of the 'breakdown' in forward bias. The construction of the curves is as follows. In reverse bias $V_{\text{dep}}$ lies on the $R_{\max}$ line. Below this the $V^{1/2}$ curve has a length dependent on $N_{\text{eff}}$ and runs to the zero voltage Ohmic curve which also depends on $N_{\text{eff}}$ through $W_0$. Running upwards in forward bias we reach $R_s$, related to the doping level of the bulk semi-conductor. Since the curves scale upwards as the density of g–r centres increases the measurement of the defect density generation with fluence, $\alpha$, is a good method except for the case shown in Fig. 1(d) and generally when the material becomes fairly relaxation-like.

In real life one is perhaps confronted with a particular experimental sample and wishes to know from the current–voltage curves what traps it contains. Usually enough is known about the dimensions and material that the expected Ohmic, maximum resistance, $R_{\max}$, line can be drawn on the experimental plot. The undepleted sample material line, $R_s$, can then be deduced from the material parameters or seen experimentally from the forward bias curves. At this stage it may be possible to deduce whether the density of g–r centres is high enough that the material needs to be considered as a relaxation-like material or simply as the combination of a diffusion and g–r current as in Eq. (11). The general shape of the curves in the relaxation region, such as the voltage at which the forward and reverse bias curves diverge, indicates whether the sample is dominated by deep acceptors or donors.

The $I$–$V$ plots derive from integrals over the whole sample and so cannot show the detail that the capacitance–voltage–frequency or charge collection data can. Even a detailed experimental set with increasing fluence cannot be easily analysed since $N_{\text{GR}}$ and $N_{\text{T}}$ are both increasing.

For the LDD and LDA the curves appear less relaxation-like since the divergence of the forward and backward curves, $V_0$, $V_t$ are all low and constant.

We have attempted curve fitting of these modelled data to obtain $V_0$ and $G_0$ using the analytic Eq. (24a) in forward bias, $R_0$ and $R_1$ using Eq. (19) in reverse bias and $V_t$ from Eq. (20) and $V_{\text{dep}}$ from the saturation point. The constants produced were of reasonable size but the fits were not good over the range of $N_{\text{GR}}$ used here except for the large DA case where the sample is well into the relaxation region. This is not unexpected since the analytic model does assume that the sample is relaxation-like. We therefore suggest that care is taken in using the fitting data and the analytic analysis here is used mainly for a good understanding of the sample physics.

## 6. Implications and applications of this understanding

It is shown that an asymmetric diode of relaxation material has an Ohmic characteristic with a resistance depending on the dimensions and the intrinsic semi-conductor properties and not on the type and details of the junction itself. In many materials it is not easy to make a 'good' electrical contact and recipes are devised to produce an Ohmic characteristic over an acceptable voltage range. It is possible that such contacts are not truly Ohmic but made to relaxation material. Thus a full current–voltage, or capacitance–voltage, analysis is needed on an asymmetric junction to determine whether a contact is really Ohmic.

It is clear that the external Ohmic characteristic hides a complex internal physical structure. There is a great difference between a semi-conductor resistor and a diode forcing its constituent semi-conductor to act relaxation-like. The current carriers are created differently and the Fermi level is in a different place. These differences must be appreciated if the device is used for more complex purposes. For example the results of a DLTS experiment depend on the excitation method and the positions of the Fermi level before and after the excitation. These are different for a relaxation diode and a lifetime diode. The appropriate analysis needs to be performed to determine the correct trap concentrations.

The above analysis indicates that this relaxation analysis needs to be applied, or at least considered, on highly defected, high resistivity material. These include irradiated, high resistivity semi-conductors, high resistivity compensated or intrinsic semi-conductors doped with lifetime killers such as Au and semi-insulating materials. In the literature on measurements in such materials, and devices made of them, very rarely is this appropriate analysis carried out but the equations and assumptions for lifetime materials are used.

Examples of common devices to which the relaxation analysis should be applied are irradiated silicon diodes made for high-energy particle detectors, Au doped diodes and semi-insulating GaAs used as a substrate for MESFETs. Proton implantation of GaAs to enhance the isolation. It is apparent that some of the effects that have been observed can only be interpreted if the present type of analysis is used. An example is the DLTS and backgating analysis of GaAsFETs. Possible uses of relaxation material are for high value resistors with well-defined resistivity and well characterised electrical isolation produced by radiation damage. For example irradiated silicon could be used as a lattice matched buried isolation layer.

We have also used this analysis to obtain results on the behaviour of these materials in capacitance–voltage experiments, in the internal field and hence charge collection in radiation detector diodes and in MESFETs made on semi-insulating substrates. We hope to present these results later.

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