ANALYTICAL MODEL TO DETERMINE PROBABILITY DENSITY FUNCTION OF AMORPHOUS SILICON WITH DANGLING BONDS AND CORRELATION EFFECT AMONG THEM

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Abstract:

The probability density function of a-Si, taking into consideration presence of dangling bonds with correlation effect, is derived . The effects of temperature, trap level positions, free carriers concentrations and ratio of capture cross sections on the probability density function have been studied with respect to various positions of donor like and acceptor like trap levels, where it is found by MATLAB that variation of position of acceptor like trap level divides the curve of probability within air gap into three sublevels of values one, zero and the third has values in between. These sublevels have been affected by increasing the temperature of a-Si wafer, changing the concentration of free carriers and position of donor like trap level, while changing of ratio of capture cross section has no effect on the distribution of probability density function.

نموذج تحليلي لتحديد دالة كثافة الاحتمالية للسليكون العشوائي بوجود الأواصر المتدلية والتأثير المتبادل بينها

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الخلاصة

تم اشتقاق معادلة دالة كثافة الاحتمالية للسليكون العشوائي أخذين بنظر الاعتبار وجود الأواصر المتدلية و التأثير المتبادل فيما بينها . ثم تم دراسة تأثير كل من درجة الحرارة و موقع مستوى الصيد وقيم مختلفة لتركيز حاملات الشحنة الحرة و نسبة المقطع الجانبي للصيد على دالة كثافة الاحتمالية نسبتا" لمواقع مختلفة لمستويات الصيد الشبيهة بالمتقبلة والشبيهة بالواهبة. وبمساعدة البرنامج MATLAB فقد تبين أن تغيير موقع مستوي الصيد الشبيه بالمتقبل أدى لتقسيم منحني دالة كثافة الاحتمالية إلى ثلاثة مستويات ، الأول قريب من حافة حزمة التكافؤ وهو ذات قيمة تساوي واحد ، والثاني قريب من حافة حزمة التوصيل وهو ذات قيمة تساوي صفر ، أما الثالث فيقع بينهما ويمتلك قيم تتغير بين الواحد والصفر . هذه المستويات تأثرت بازدياد درجة الحرارة و تغير تركيز حاملات الشحنة الحرة وتغير موقع مستوي الصيد الشبيه بالمتقبل ، بينما لم يظهر أي تأثير لتغير نسبة القطع الجانبي للصيد على منحني الدالة .

Introduction:

The structure of amorphous silicon, a-Si, characterizes by presence of high density of states in the gap between conduction and valance bands. Those states act as traps or generation - recombination centers. So the concentrations of captured carriers in a-Si is much greater than concentrations of free carriers [Madan ,1976]. Therefore, in contrast with single crystalline silicon, the conduction band and valance band in a-Si are not separated by clearly defined energy gap, where the acceptor like and donor like states are tailing in that gap and overlapping approximately in the middle of gap [Madan ,1976].

Many experiments had been achieved to determine style of proper distribution of that states within the gap. The model of most compatible experimental results with practical events was the distribution model suggested by Hack, Guha and Shur , where the density of acceptor like states $g_A(E)$ and donor like states $g_D(E)$ are described by the given functions [Hack,1985] :

$$g_A(E) = A_{ct}.\exp(E - E_c)/w_c \qquad \text{... (1)}$$

$$g_D(E) = A_{vt}.\exp(E_v - E)/w_v \qquad \text{... (2)}$$

Where A_{ct} and A_{vt} are the concentration of acceptor like and donor like states at the edges of conduction and valance bands respectively .

The electrical properties of a-Si and its electronic structure are greatly affected by the distribution of those states and their cases, if they were empty or occupied by carriers [Balberg,2001]. The occupation of states is governed by Fermi – Dirac distribution [Madan ,1976]. Out of thermal equilibrium, occupation of states is strongly related to the dynamic of thermal generation – recombination rate of charge carriers [Furlan,1987].

Mathematically , the occupation of acceptor and donor like states in undoped a-Si are described by the following equations, called the occupancy density functions related to acceptor and donor like states , f_{tA} and f_{tD} , respectively [Furlan,1987] :

$$f_{tA} = \frac{R_A p_1 + n}{R_A(p + p_1) + n + n_1} \qquad \text{... (3)}$$

$$f_{tD} = \frac{R_D n + p_1}{R_D(n + n_1) + p + p_1} \qquad \text{... (4)}$$

Where n , p are the concentration of free carriers, p_1 and, n_1 are concentration of captured carriers with respect to a certain G – R center related to the intrinsic Fermi level.

In amorphous semiconductors, defects are of different kinds as compared to crystalline materials, the main defects are those related to the deviations from the average coordination number, bond length and bond angle, which will cause disorder in stracture of amorphous silicon [Yacobi, 2004]. Due to this disorder, the concentration of dangling bonds normally rises, those dangling bonds occur when silicon atom does not bond to four neighboring atoms [6] .

The presence of dangling bonds widely affects the distribution of states densities in a-Si and badly affects the properties of amorphous silicon [**Fritzsche**,1977] . To study effect of dangling bonds , they are represented by different mathematical formulas . The representation adopted by al-samrai is also adopted here, where the bonds are given by peaks of fixed amplitude , A_a and A_p , and fixed width ΔE [AL – Samarai,1989].

Many studies have been achieved to overcome the problems related to defects produced due to presence of dangling bonds in structure of a-Si, the most important method in this field that suggests doping the a-Si with some concentration of hydrogen to produce the hydrogenated amorphous silicon a-Si:H [Feldmam,2004], and the more recent method is that depending on Germanium - induced perimeter to get crystallized a-Si [Hakim ,2007].

Theory

In the energy gap, there are the density of positive ions which are equal to density of empty donor like states $G_{tD} - g_{tD}$, the density of negative ions which are equal to density of occupied acceptor like states g_{tA}, and the neutral atoms which are equal to density of empty acceptor like states $G_{tA} - g_{tA}$, where G_{tD} and G_{tA} represents the total concentrations of donor like and acceptor like states, empty plus occupied, in presence of dangling bonds with correlation effect among them .

So the overall concentrations of states is given by :

$$G_t = (G_{tD} - g_{tD}) + g_{tA} + (G_{tA} - g_{tA}) \quad \dots (5)$$

which can be rewritten as :

$$G_t = G_{tA} + G_{tD} - g_{tD} \quad \dots (6)$$

The probability density function of acceptor like states in presence of dangling bonds and correlation effect , F_{tA} , represents the ratio of concentration of occupied acceptor like states , g_{tA} , to the total concentration of states G_t ,[Montgomery,2003] :

$$F_{tA} = \frac{g_{tA}}{G_t} \quad \dots (7)$$

which can be found equal to :

$$F_{tA} = \frac{1}{1 + \frac{n_{1A} + R_A P}{n + R_A P_{1A}} + \frac{P + R_D n_{1D}}{P_{1D} + R_D n} \cdot \frac{n_{1A} + R_A P}{n + R_A P_{1A}}} \quad \dots (8)$$

While the probability density function of donor like states in presence of dangling bonds and correlation effect , F_{tD} , represents the ratio of concentration of occupied donor like states , g_{tD} , to total concentration G_t ,[Montgomery,2003] :

$$F_{tD} = \frac{g_{tD}}{G_t} \quad \dots (9)$$

which can be found equal to :

$$F_{tD} = \frac{1}{1 + \frac{P + R_D n_{1D}}{P_{1D} + R_D n} + \frac{n + R_A P_{1A}}{n_{1A} + R_A P}} \quad \dots (10)$$

Where n_{1A} , P_{1A} are the concentrations of captured carriers with respect to acceptor like trap level , n_{1D} , P_{1D} are the concentrations of captured carriers with respect to donor like trap level and R_A , R_D are the capture cross section ratios with respect to acceptor like and donor like states respectively .

The Results :

The probability density functions of amorphous silicon , a-Si , with dangling bonds and correlation effect among them, is studied through four obtained curves for F_{tA} using MATLAB, the first curve is for variation of probability density function of a-Si , F_{tA} , with position of acceptor like trap level E_{tA} for different values of free carriers concentrations *n* and p at certain donor like trap level, the second is for variation of F_{tA} with position of acceptor like trap level E_{tA} for various positions of donor like trap levels at certain concentration of free carriers, the third is for variation of F_{tA} with acceptor like trap level E_{tA} for different values of temperature and the fourth is for variation of F_{tA} with position of acceptor like trap level E_{tA} for different values of captured cross section ratios R_A and R_D .The calculations were performed regarding the value of intrinsic concentration $n_i = 1.9 \times 10^5$ cm^{-3} , ratios of capture cross section $R_A = R_D = 100$, temperature T = 25 C^0 and position of Fermi level E_i = 0.8 ev. **Figures (1)** through **(4)** show the results of those studies, where:

1. **Figure(1)** , shows that variation of probability density function FtA through the gap , between conduction and valance bands , with position of acceptor like trap level, EtA , and the donor like trap level is at position EtD=0.4ev, it is found that the probability density function can be divided into three sub regions , the first is that close to valance band where value of FtA is very close or equal to one , the second is that close to position of intrinsic Fermi level (Ei) where the values of FtA sharply drop to zero to form the third region which close to conduction band .

2. If the curves of **Figure(1)** are compared with similar curves obtained by Furlan [4] for a-si without dangling bonds , it shows that presence of dangling bonds , with correlation effect , makes the second region very narrow , that beyond to presence of dangling bonds and correlation effect where that effect will lead to increase the density of defects. This explains the reason of bad effect of correlation effect among dangling bonds on photoconductivity of a-si where Taylor and Simmon [1972] had been mentioned that the majority of generation - recombination rate has been taken place in this region .

3. **Figure(1)** shows, too ,that the first and third regions widths vary with variation of free carriers concentrations , n and p , where more concentrations of free carriers mean less concentrations of captured carriers and vise verse , which also means less or more occupation of captured levels effecting values of FtA and FtD .

4. **Figure(2)** shows variation of probability density function FtA with position of acceptor like trap level EtA for three positions of donor like trap levels EtD 0.2ev, 0.6ev and 1.0ev . By this figure, it is clear that the donor like trap level at position 1.0ev, has no effect on probability density function (FtA) because this position of EtD is above Fermi level (Ei = o.8ev approximately) where the normal and effective position to EtD is below Ei , while for values of EtD less than Ei, gives us a hint that decreasing of EtD leads to corresponding decrease in the region of FtA equal to one, where less value for position of donor like trap level EtD means that the donor like trap level is much closer to valance band making it in higher activity to trap the electrons and holes of that band .

5. **Figure(3)** , shows variation of probability density function FtA with the position of acceptor like trap level EtA for three different values of temperature , T . It is found that increasing the temperature of a-Si wafer improves its properties by making the structure of wafer approaches to crystallization [Mullin,2001]. So, as temperature increases in **Figure(3)**, the second sublevel becomes wider, which is an essential region in the gap of amorphous silicon because the majority of generation recombination process has been taken place in this region .

6. By **Figure(4)**, effect of changing the ratios of captured cross section , RA and RD on probability density function FtA, is studied , where FtA via EtA was plotted for three different values of RA and RD and it was expected to get three different curves for FtA but it is found only one, which means that varying the value of RA or RD has no effect on FtA . That beyond to increasing of defects due to the bad effect of dangling bonds and correlation effect among them, which will lead to cancel the second region , where the effect of changing RA or RD on FtA is expected to be noticed . This result has been enhanced mathematically by partial derivative of FtA with respect to capture cross section ratio RA ($\partial F_{tA} / \partial R_A$) which found equal to zero .

   Similar result was deduced by Furlan [1987] when he studied the probability density function in undoped amorphous silicon, without dangling bonds, where he mentioned that "changing in captured cross sections ratios RA or RD will only affect the width of second region". Here, as the width of second region, is drastically eliminated , nearly to zero, so it is acceptable to say that RA or RD has no effect on probability density function .

Conclusions:

1. Increasing the doping of a-Si wafer will shift the curve of probability function toward conduction band, causing in making the region of F_{tA} =1 wider, this beyond to the fact that doping can control the position of Fermi level .
2. As the position of donor like trap level E_{tD} moves to be closer to conduction band, the curve of probability density function shifts toward the valance band where the empty acceptor like trap states increases .
3. Rising the temperature of amorphous silicon wafer will effect the width of middle region making it wider and decreasing the width of first and third regions.
4. Changing the ratio of capture cross section has no effect on the probability density function of amorphous silicon.
5. In general, presence of dangling bonds with correlation effect among them will badly affect the properties of amorphous silicon by affecting the width of middle region of probability density function which play an important rule in determining the properties of a-Si because most of generation recombination process has taken place in this region.

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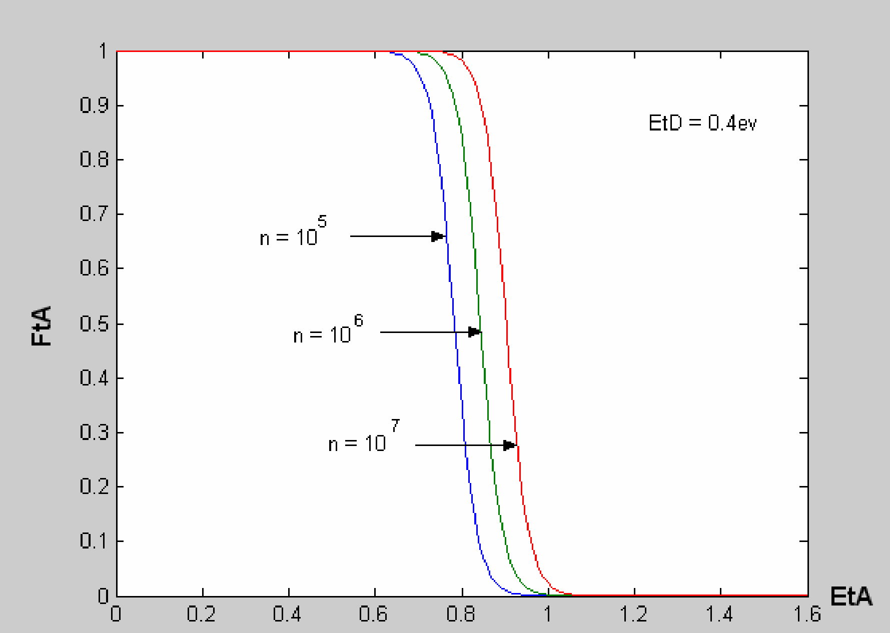

Fig.(1) Variation of FtA with EtA for different concetrations of free carriers.

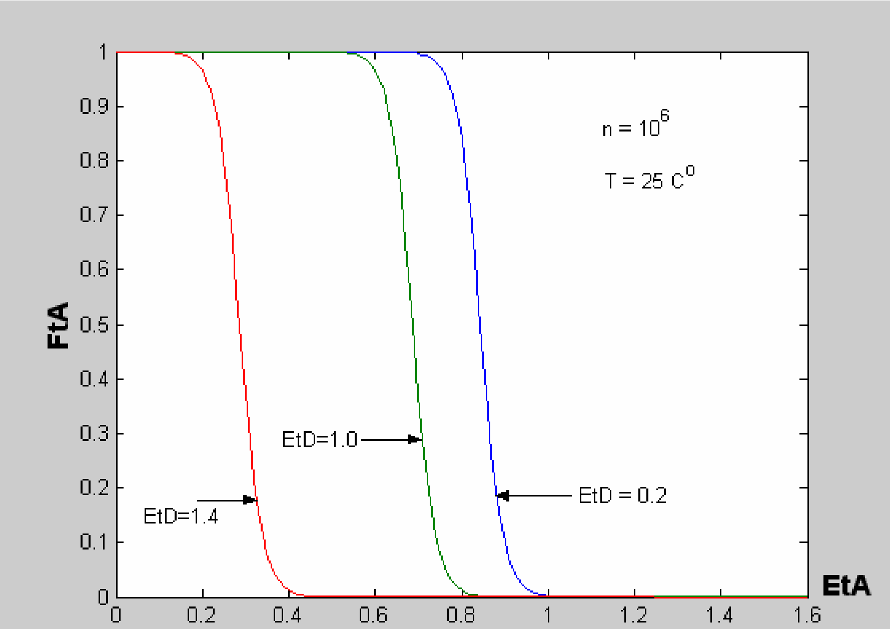

Fig.(2) Variation of FtA with EtA for various positions of donor like trap level.

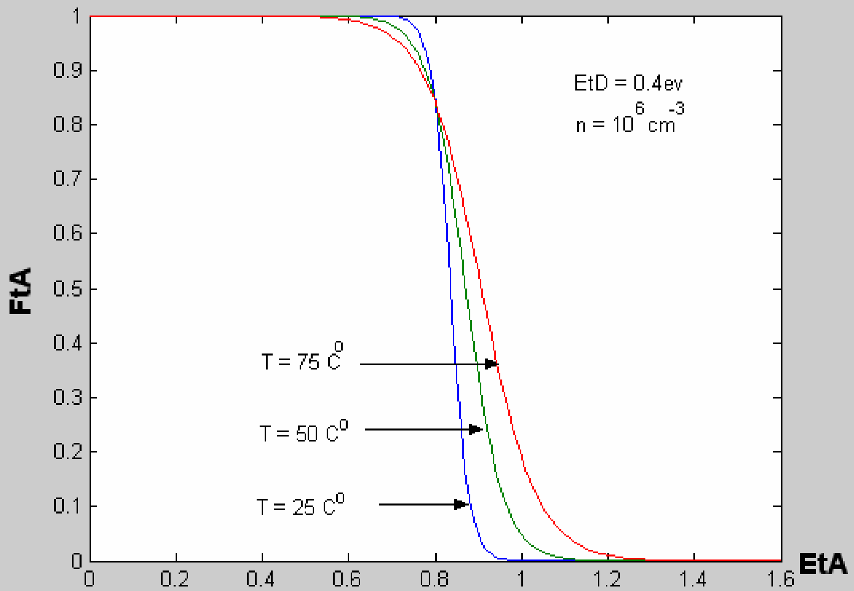

Fig.(3) Variation of FtA with EtA for different values of temprature T.

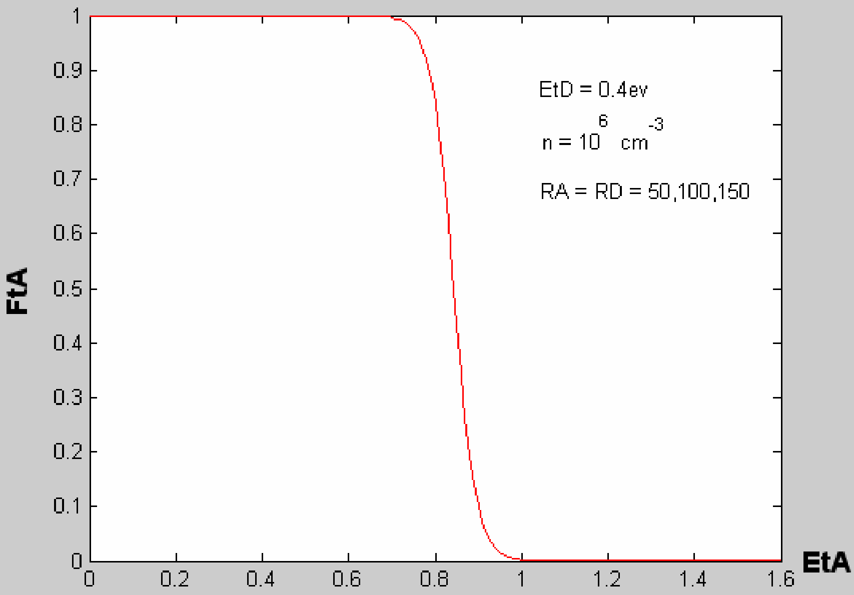

Fig.(4) Variation of FtA with EtA for three different values of RA and RD