Strujno – naponske karakteristike CNT FETova

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U ovom radu ispitivane su karakteristike FETova izrađenih na bazi ugljeničnih nanotuba (CNT FETova). U prvom delu rada, predstavljene su neke osnovne osobine ugljeničnih nanotuba. Zatim je razvijen analitički model strujno – naponskih karakteristika CNT FETova koji dobro opisuje ponašanje ove savremene nanoelektronske naprave. Na bazi predloženog modela urađene su simulacije. Dobijeni rezultati su u saglasnosti sa prethodno publikovanim.

Ključne reči: *CNT FET, strujno – naponske karakteristike, analitički model*

1. UVOD

Trendovi u mikroelektronici su usmereni ka povećavanju gustine pakovanja komponenti u čipu, što vodi povećanju brzine rada naprava i istovremenom obezbeđivanju mogućnosti izvršavanja složenijih funkcija [1, 2]. Pritom se vodi računa o zahtevima potrošača za što kvalitetnijim, pouzdanijim i multi-funkcionalnim napravama.

U cilju poboljšavanja karakteristika, traže se nova rešenja u koja svakako spada korišćenje novih materijala i struktura. Jedno od veoma dobrih novih rešenja predstavlja korišćenje silicijum karbida (SiC), umesto standardnog silicijumskog materijala [3 - 7], čime se dobijaju elektronske komponente koje mogu da rade na znatno višim tempertaturama, sa višim učestanostima i sl. Ovakva istraživanja vodila su ka početku korišćenja ugljenika, odnosno ugljeničnih nanotuba (carbon nanotubes – CNTs), kao materijala za realizaciju elektronskih naprava.

Više od decenije, nanomaterijali, u koje spadaju i ugljenične nanotube, proučavani su i istraživani u mehanici, fizici, hemiji, fotonici, elektronici. Njihovim daljim razvojem tek treba da dođe do brojnih otkrića koja bi dovela i do primene u komercijalne svrhe.

Ugljenične nanotube privlače dosta pažnje zbog svojih izvanrednih električnih, toplotnih i mehaničkih osobina i širokog opsega potencijalnih primena. Kontrola kvaliteta CNTa se konstantno povećava jer čistoća, defekti, prečnik i dužina nanotube direktno utiču na njena konačna svojstva. Nažalost, dosadašnji rezultati dosta odstupaju od željenih, pa je dobijanje visokokvalitetnih ugljeničnih nanotuba i dalje problem koji tek treba da se reši.

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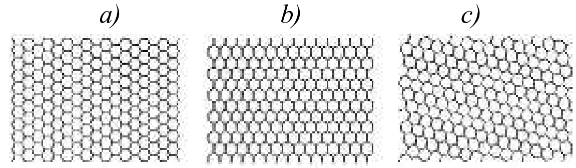
2. UGLJENIČNE NANOTUBE

CNT su cilindrični molekuli izgrađeni od šestougaonih struktura hibridizovanih ugljenikovih atoma. Pripadaju familiji fulerena, alotropskih modifikacija ugljenika [8]. Opisuju se kao šuplji cilindri koji nastaju kotrljanjem pojedinačnih ili većeg broja slojeva grafena u bezšavne cilindre (slika 1).

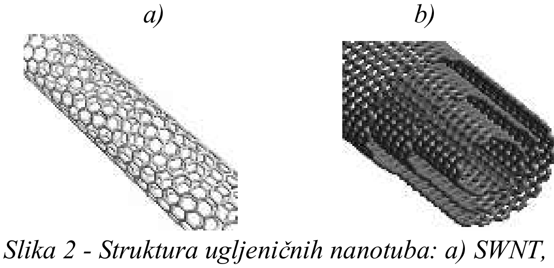
a) *b)* *c)*



Slika 1 - Listovi grafena koji pokazuju orijentaciju grafenskih heksagona a) fotelja, b) cik-cak, c) spiralni

Postoje dve vrste nanotuba: jednozidne nanotube (*single-walled carbon nanotubes, SWNTs*) i višezidne nanotube (*multi-walled carbon nanotubes, MWNTs*) koje u svom sastavu imaju i do deset koncentričnih cilindara SWNTs (slika 2). MWNTs imaju veći spoljni prečnik, česte strukturne defekte i manje stabilnu nanostrukturu. Zbog toga su se jednozidne nanotube pokazale kao pogodnije za praktičnu primenu.

a) *b)*



Slika 2 - Struktura ugljeničnih nanotuba: a) SWNT, b) MWNT

Poboljšanje tehnika sinteze CNTa radi se u cilju povećanja kvaliteta i obezbeđivanja mogućnosti kontrole njihovih dimenzija. Osnovni način sintetisanja

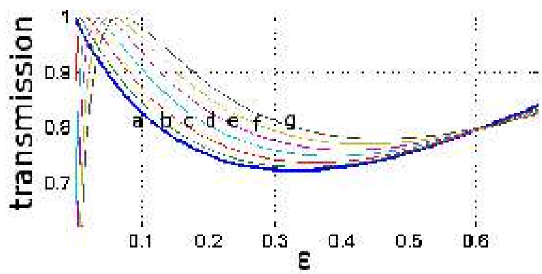


Fig. 8. Curves are plotted for n = 1: a) Δ = π, b) Δ = = π − 0,02, c) Δ = π − 0,05, d) Δ = π − 0,09, e) Δ = π−0,13, f) Δ = π−0,17, g) Δ = π− 0,21

Fig.8 shows the evolution of transmission when the parameter Δ takes the highest possible values. Contrary to the case of small Δ, here we obtain a usual graph of transmission. In addition, it is obvious that for increased Δ, the transmission curve approaches the ordinate.

An analysis similar to the one presented here for quantum wells may be used to show that the second order maxima do not appear in case of electron transmission through the potential barrier.

SUMMARY AND CONCLUSIONS

In this paper, we provide a detailed investigation of the dependence of transmission on electron energy in rectangular semiconductor quantum well. It is shown that, in the given model, there appear two types of maxima of transmission:

a) first order maxima, with transmission equal to 1. There is an infinite number of these maxima regardless of the value of quantum well strength
b) second order maxima (and corresponding second order minima), with transmission less than 1. Their existence depends on the strength of the quantum well.

It has been proven analytically that there exists an infinite number of intervals (with finite widths) of quantum well strength, in which the second order maxima occur. The widths of these intervals increase as the order of the quantum well strength increases, and tend asymptotically to $\frac{\pi}{4}-\frac{1}{2}\approx 0.285$. It should be noted that the second order maxima occur at low energies, lower than any energy of first order maxima, which justifies the assumption of uniform effective mass.

Further work will entail an analysis of transmission in semiconductor quantum wells where the difference between effective masses in the well and the barrier region cannot be neglected. Similar procedure will be applied to photonic heterostructures (analogous to quantum wells) where the absorption occurs as well as the transmission.

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REZIME

ANALIZA SPECIFIČNIH MAKSIMUMA TRANSMISIJE KROZ PRAVOUGAONU POLUPROVODNIČKU KVANTNU JAMU

U ovom radu posmatraćemo koeficijent transmisije kroz pravougaonu jamu, kada su efektivne mase elektrona van i unutar kvantne jame jednake i ne zavise od položaja. Pokazano je da postoji beskonačan broj konačnih intervala intenziteta kvantne jame za koje postoje maksimumi manji od jedinice. Pored toga pokazano je i da za velike vrednosti intenziteta kvantne jame veličina ovih intervala ima asimptotsku vrednost. Takođe, detaljno je analizirana zavisnost transmisije elektrona od energije u slučaju kada je intenzitet kvantne jame približno jednak celobrojnom umnošku broja π.

Ključne reči: *transmisija, poluprovodnička kvantna jama, intenzitet kvantne jame, maksimumi prvog reda, maksimumi drugog reda.*

can be approximated by the expression: $\varepsilon_{z,n} = \frac{1}{n\pi}$, which implies $\frac{1}{(n+1)\pi} < \varepsilon_{0,n} < \frac{1}{n\pi}$. This further leads to:

$$\frac{1}{\varepsilon_{0n}} = n\pi + \xi_n \ , \ \xi_n \in [0,\pi) \tag{12}$$

It allows us to express equation (9) in the form:

$$tg\left(\xi_n - \frac{1}{2} + \sum_{i=1}^{+\infty} \frac{a_i}{(n\pi + \xi_n)^i}\right) = 1 + \sum_{i=1}^{+\infty} \frac{b_i}{(n\pi + \xi_n)^i} \tag{13}$$

If we neglect the terms $\frac{1}{n\pi + n}$, $\frac{1}{(n\pi + n)^2}$,…. for high values of parameter n, we obtain the following expression for ξ:

$$\xi_\infty = \frac{\pi}{4} + \frac{1}{2};$$

and

$$\varepsilon_{0\infty} \to \frac{1}{n\pi + \xi_\infty} \tag{14}$$

In case that we maintain the same order of approximation, Δ_{th} (for infinite value of parameter n) becomes:

$$\Delta_{th,\infty} \approx \frac{1 - \varepsilon_{0\infty}}{\varepsilon_{0\infty}} - n\pi = \frac{\pi}{4} - \frac{1}{2} \tag{15}$$

By considering higher order approximation, the quantity ξ can be written as:

$$\xi_{na} = \xi_\infty - \frac{1}{8\theta_n}\left(1 - \frac{61}{8\theta_n}\right) + O\left(\frac{1}{\theta_n^3}\right) \tag{16}$$

$$\theta_{na} = n\pi + \xi_\infty, \ \delta_{na} = -\frac{1}{8\theta_n}\left(1 - \frac{61}{8\theta_n}\right)$$

In Table 2, the ratios of exact values of δ_n and the ones calculated from formula (16) are given. It can be seen that the asymptotic expression (16) for $n > 7$ leads to an error of less than 5%, and for $n = 10$, this error is less than 2% (see Table 2).

It can be shown that in the asymptotic case, an analogous expression for Δ_{th} reads:

$$\Delta_{th,na} = \Delta_{th,\infty} - \frac{5}{8\theta_n} + \frac{29}{64\theta_n^2} + O\left(\frac{1}{\theta_n^3}\right) \tag{17}$$

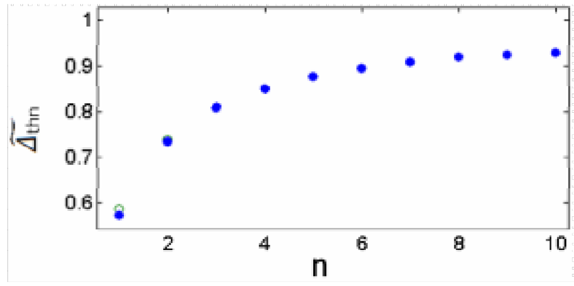


Fig. 6. Dependence normalized value $\overline{\Delta_{th,n}} = \frac{\Delta_{th,n}}{\Delta_{th,\infty}}$ on strength of quantum well order (n) $\Delta_{th\infty} = \frac{\pi}{4} - \frac{1}{2}$. Filled points correspond to exact values of $\overline{\Delta_{th,n}}$, and empty points to approximated values.

In Table 2, the ratio between $\Delta_{th,n}$ calculated from formula (17) and the correct value of $\Delta_{th,n}$, is given as well. The table shows that the approximate expression provides very accurate results. For $n = 1$ the error is 2.5%, and for $n = 3$ the error is already less than 0.2%, while for $n = 10$ it drops below 0.01% (see Table 2).

In Fig 6. we see the dependence of the parameter Δ_{th} on the order (n) of the quantum well strength.

Fig. 7. provides the best illustration of the effect under consideration. We have shown that the second order maxima exist for low values of parameters ε and Δ (Fig.7). When $\Delta = 0$, the transmission starts from 1, but as we increase Δ, the maxima lower than 1 become evident. When we reach the threshold value $\Delta = \Delta_{th}$, the extremum is degenerated to an inflection point. If we continue to increase Δ, the effect vanishes, and we obtain a conventional graph of transmission without maxima of the second order.

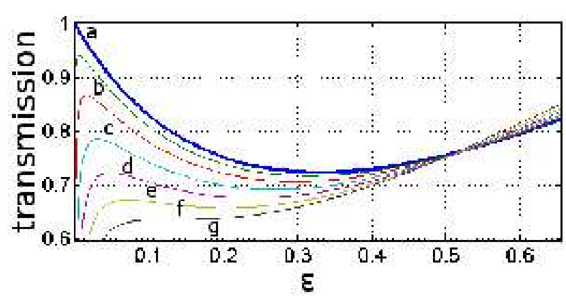


Fig. 7. Transmission for a different values of Δ for n=2. Curves on the graph are plotted for appropriate values of Δ: a) Δ=0, b) Δ=0,2, c) Δ=0,5, d) Δ=0,09, e) Δ=0,13, f) Δ=0,17, g) Δ_{th}=0,21

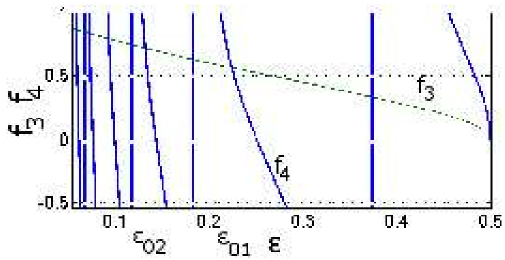


Fig. 5. Dependences $f_3(\varepsilon) = tg\frac{\sqrt{1-\varepsilon_0-2\varepsilon_0^2}}{\varepsilon_0}$ *and*

$$f_4(\varepsilon) = \frac{\sqrt{1-\varepsilon_0-2\varepsilon_0^2}}{1+2\varepsilon_0}$$

We will mark the left side of equation (9) as $f_3(\varepsilon)$, and the right side as $f_4(\varepsilon)$. From the above expressions we arrive to the condition: $0 \le \varepsilon_0 \le 0.5$, for any value of the parameter n. Equation (9) has only one unknown variable ε_0, and an infinite number of solutions ($\varepsilon_{00}, \varepsilon_{01}, \varepsilon_{02}$ ...), that corresponds to energies at which f_1 and f_2 touch each other, for certain n (ε_{00} corresponds to $n=0$, , ε_{01} corresponds to $n=1$, etc.) For $n=0$, the appropriate energy is $\varepsilon_{00}=0.5$ and $\Delta_{th}=0$, i.e. there is no quantum well. In other words, the quantum well reduces to a homogeneous semiconductor. For any other value of the parameter n ($n = 1, 2, 3$) $\varepsilon_{0,n} < 0.5$ and $\Delta_{th,n}$ is finite, as illustrated in Fig.5.

NUMERICAL RESULTS

The most important objective of this section is to determine the numerical values of the strength of the quantum well for which the second order maxima of transmission occur. We shall define new parameters:

$$\Delta_{th,\infty} = \lim_{n\to\infty} \Delta_{th,n} = \frac{\pi}{4} - \frac{1}{2}, \quad \overline{\Delta_{th,n}} = \frac{\Delta_{th,n}}{\Delta_{th,\infty}}.$$

Dependences of $\overline{\Delta_{th,n}}$ and $\overline{\Delta_{th,na}}$ on n are illustrated in Fig.6, and we observe that for $n \ge 3$ these two quantities have almost the same values (Table 2).

Table 1. Dependences $\overline{\Delta_{th,n}}$ $(\overline{\Delta_{th,n}} = \frac{\Delta_{th,n}}{\Delta_{th,\infty}})$ *and* $\varepsilon_{0,n}$ *on strength of quantum well order, calculated by formulae (1.9) and (1.10)*

n	1	2	3	4	5	6	7	8	9	10
$\overline{\Delta_{th,n}}$	0,5722	0,7348	0,8079	0,8494	0,8762	0,8949	0,9086	0,9192	0,9243	0,9290
$\varepsilon_{0,n}$ [x10^{-3}]	224,57	132,11	93,40	72,22	58,86	49,67	42,97	37,86	33,83	30,58

Table 2. Dependences $\frac{\delta_{na}}{\delta_n}$ *and* $\frac{\Delta_{th,na}}{\Delta_{th,n}}$ *on strength of quantum well order.* δ_{na} *and* $\Delta_{th,na}$ *are approximated values calculated by formulae (2.6) and (2.7), while* δ_n *and* $\Delta_{th,n}$ *are exact values calculated by formulae (1.9) and (1.10).*

n	1	2	3	4	5	6	7	8	9	10
$\frac{\delta_{na}}{\delta_n}$	0.7882	0.1426	1.0582	1.0144	1.0045	1.0009	0.9994	0.9987	0.9983	0.9981
$\frac{\Delta_{th,na}}{\Delta_{th,n}}$	1.02473	1.00488	1.00181	1.00089	1.00051	1.00032	1.00022	1.00016	1.00012	1.00009

In Table 1, values of $\overline{\Delta_{th,n}}$ for the appropriate n are presented, as well as the corresponding intersection points $\varepsilon_{0,n}$.

The roots of the function $f_3(\varepsilon_0)$, which reads

$$f_3(\varepsilon_0) = tg\frac{\sqrt{1-\varepsilon_{0n}-2\varepsilon_{0n}^2}}{\varepsilon_{0n}}$$, are at energies ε_{zn}:

$$\varepsilon_{zn} = \frac{\sqrt{9+4(n\pi)^2}-1}{2(n\pi)^2+4}, \quad n = 1,2,3 \ldots \qquad (11)$$

while for $n=0$, $\varepsilon_{z0} = 0.5$. The solution of equation $f_3(\varepsilon_{0n}) = f_4(\varepsilon_{0n})$, lies in an interval defined by the roots $\varepsilon_{z,n}$ and $\varepsilon_{z,n+1}$, hence $\varepsilon_{z,n+1} < \varepsilon_{0,n} < \varepsilon_{z,n}$. In case when parameter n obtains large values, roots

$\theta(\varepsilon)$ belongs to the interval $\left[(n\pi+\Delta),(n+1)\pi\right]$, and $f_1(\varepsilon)$ has a vertical asymptote within [0, $\varepsilon_{max\,1}$] (Fig. 3b). If we denote the energy position of this asymptote as $\varepsilon=\varepsilon_{va}$, then for $\varepsilon>\varepsilon_{va}$ we have $f_1(\varepsilon)<0$ and equation (6) has no solution therein.

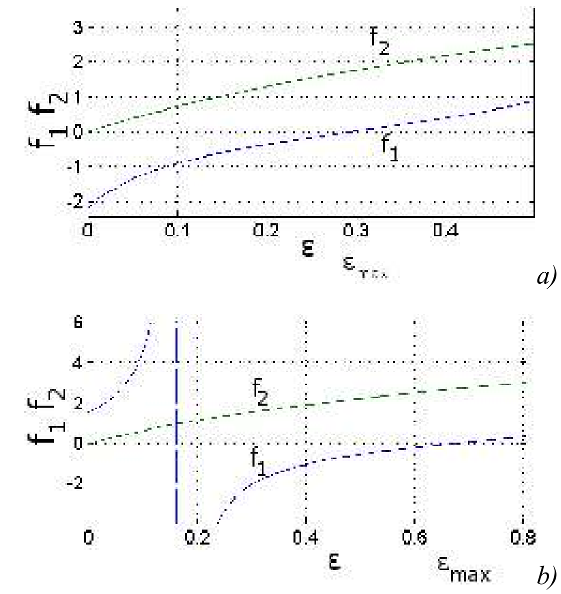
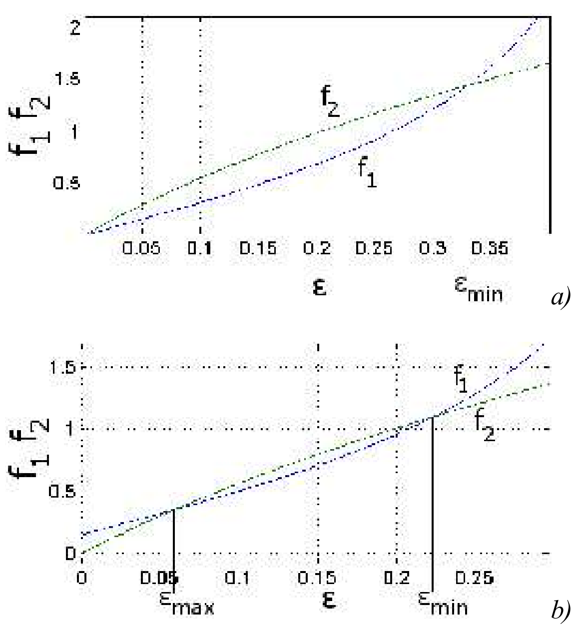


Fig.3. Dependence of $f_1(\varepsilon)$ i $f_2(\varepsilon)$, for $\varepsilon<\varepsilon_{\max 1}$ and n=2. a) Δ=2,(Δ> $\frac{\pi}{2}$) and b) Δ=1,(Δ< $\frac{\pi}{2}$) In first case f_1 and f_2 do not have any intersection points, in second we see that for $\varepsilon>\varepsilon_{va1}$ there is no intersection points



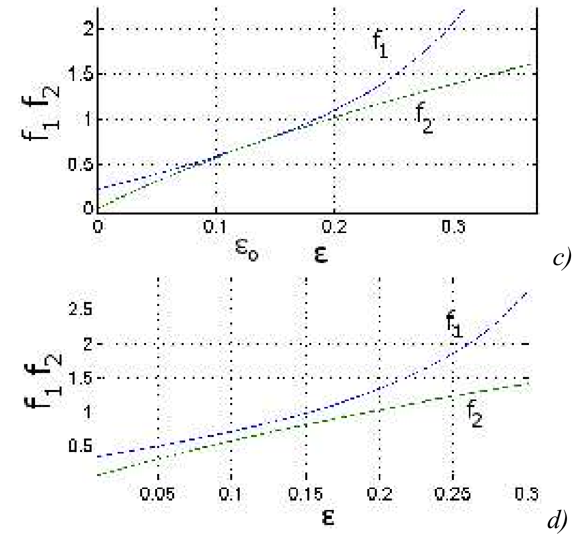


Fig. 4. Dependences $f_1(\varepsilon)$ and $f_2(\varepsilon)$; n = 2, for a) Δ=0, b) Δ=0.15, c) $\Delta=\Delta_{th}\approx 0.21$, d) Δ=0.3.

If $\Delta=0$, then the functions f_1 and f_2 intersect at $\varepsilon=0$ and $\varepsilon=\varepsilon_{\min}$. It has already been shown that for $\varepsilon=0$ there is no extreme value, while the second intersection point corresponds to a minimum of transmission $T(\varepsilon)$ (Fig. 4a).

With increasing Δ, the functions f_1 and f_2 intersect at two points, the lower of which corresponds to a maximum, while the other one corresponds to a minimum (Fig. 4b). Further increase of Δ reduces the distance between these two intersection points, until they coincide at $\Delta=\Delta_{th}$ (Fig. 4c.). For even higher Δ ($\Delta>\Delta_{th}$), functions f_1 and f_2 cease to have any intersection points (Fig. 4d).

At the point of contact we clearly have $f_1(\varepsilon_0)=f_2(\varepsilon_0)$, but also $f_1'(\varepsilon_0)=f_2'(\varepsilon_0)$. In explicit form these conditions read:

$$tg\left[(n\pi+\Delta_{th})\sqrt{1+\varepsilon_0}\right]=\frac{(n\pi+\Delta_{th})\varepsilon_0\sqrt{1+\varepsilon_0}}{1+2\varepsilon_0} \qquad (7)$$

$$\frac{1}{\cos^2((n\pi+\Delta_{th})\sqrt{1+\varepsilon_0})}=\frac{2\varepsilon_0^2+3\varepsilon_0+2}{(1+2\varepsilon_0)^2} \qquad (8)$$

The system of equations (7-8) can be written in a more suitable form:

$$tg\frac{\sqrt{1-\varepsilon_0-2\varepsilon_0^2}}{\varepsilon_0}=\frac{\sqrt{1-\varepsilon_0-2\varepsilon_0^2}}{1+2\varepsilon_0} \qquad (9)$$

$$\Delta_{th}=\frac{\sqrt{1-\varepsilon_0-2\varepsilon_0^2}}{\varepsilon_0\sqrt{1+\varepsilon_0}-n\pi} \qquad (10)$$

The dimensionless quantity q can be written in a more practical form: $q = 0.51\sqrt{m^*_w U_0(eV)}d\left[\dot{A}\right]$, with $m_w^* = m_w / m_0$ (m_0 is the free electron mass). In $GaAs / Al_x Ga_{1-x} As$ quantum wells we obtain $\sqrt{m_w^* U_0} \sim 0.1$, and the width d takes values from around 20 $\dot{A}$ to 200 $\dot{A}$, so q lies approximately within the interval (0.5, 5). This interval may be significantly wider for quantum wells based on other semiconductor materials, so in the theoretical analysis we will consider the limit $q \in [0,+\infty)$, and for energies $\varepsilon \in [0,+\infty)$. It is convenient to write q in the form:

$q = n\pi + \Delta$, where $n = 0,1,2...$

and $\Delta \in [0,\pi)$.

Prior to finding the extrema of transmission, we will analyze $T(\varepsilon)$ and $\frac{d}{d\varepsilon}T(\varepsilon)$ for $\varepsilon = 0$. If $q \neq n\pi$ then $T(0) = 0$, while $\frac{d}{d\varepsilon}T(\varepsilon)\Big|_{\varepsilon=0} = \frac{4}{\sin^2 q}$. On the other hand, for $q = n\pi$, the transmission at $\varepsilon = 0$ is $T(0) = 1$ and $\frac{d}{d\varepsilon}T(\varepsilon)\Big|_{\varepsilon=0} = -\frac{n^2\pi^2}{16}$. This proves the absence of extrema for the lowest energy ($\varepsilon = 0$) regardless of the q value.

Extreme values of $T(\varepsilon)$ are determined from the equation:

$$\frac{dT(\varepsilon)}{d\varepsilon} = 4\frac{\sin\theta\left[(2\varepsilon+1)\sin\theta - q\varepsilon\sqrt{\varepsilon+1}\cos\theta\right]}{(4\varepsilon(\varepsilon+1)+\sin^2\theta)^2} \quad (3)$$

$$\theta = (n\pi + \Delta)\sqrt{1+\varepsilon}$$

which has two groups of solutions.

The first group of solutions is found from the condition:

$$\sin\theta = \sin\left[(n\pi + \Delta)\sqrt{1+\varepsilon}\right] = 0 \quad (4)$$

From (1.4) we have $\varepsilon_{max1} = \left(\frac{l\pi}{n\pi + \Delta}\right)^2 - 1$, $l = n+1, n+2...$, and inserting into (2) shows that these maxima provide unity transmission $(T(\varepsilon_{max1})$. They are denoted as the first order maxima.

The second group of solutions of Eq. (3) is obtained from the condition:

$$(2\varepsilon + 1)\sin\theta - \varepsilon\theta\cos\theta = 0 \quad (5)$$

namely:

$$tg((n\pi + \Delta)\sqrt{1+\varepsilon}) = \frac{(n\pi + \Delta)\varepsilon\sqrt{1+\varepsilon}}{2\varepsilon + 1} \quad (6)$$

The solutions of this transcendent equation encompass both the energies of minima of $T(\varepsilon)$, and the second order maxima (with transmission less than one), provided that the latter occur. The left side of equation (6) will be marked as $f_1(\varepsilon, n, \Delta)$, and the right side as $f_2(\varepsilon,n,\Delta)$. The function $f_2(\varepsilon,n,\Delta)$ increases monotonically for every ε, regardless of the values of n and Δ. Next, we will consider the energies from the interval $\left[\varepsilon_{max1},+\infty\right)$, where $f_2(\varepsilon,n,\Delta)$ is always positive, and ε_{max1} represents the first maxima of the first order:

$$\varepsilon_{max1} = \left(\frac{n+1}{n\pi + \Delta}\right)^2 \pi^2 - 1.$$

For $\varepsilon = \varepsilon_{max1}$, $f1(\varepsilon = \varepsilon_{max1}) = 0$, and with increasing energy, f_1 increases to infinity and intersects with f_2 at a certain value of energy. This intersection point will be denoted as ε_{max1} (Fig 2.). If we continue to increase the energy, f_1 reaches its vertical asymptote after which it becomes negative and starts to rise again, attaining zero value at $\varepsilon = \varepsilon_{max2}$. This is the energy of the second maxima from the first order solutions set. Given that f_1 is a periodic function of θ, the previous analysis can be extended to conclude that, starting from the energy ε_{max1}, the first order maxima and the minima of transmission occur alternately.

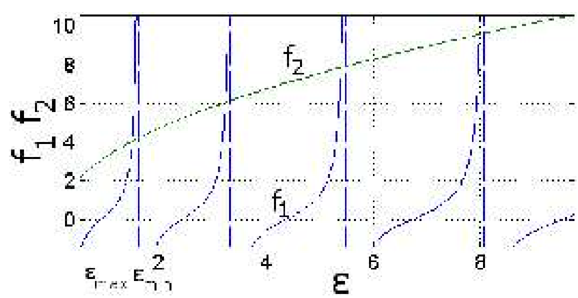


Fig.2. Dependence of $f_1(\varepsilon)$ and $f_2(\varepsilon)$ for $n = 2, \Delta = 0{,}5$ and energies $\varepsilon > \varepsilon_{max1}$.

Now we will analyze the energy interval $(0, \varepsilon_{max1})$.

If $\Delta \in \left[\frac{\pi}{2},\pi\right]$, then $\theta(\varepsilon)$ belongs to the interval $\left[(n\pi + \Delta),(n+1)\pi\right]$ and $f_1(\varepsilon)$ is negative for all relevant values of energy ε, which implies that (6) has no solution (Fig.3a). On the other hand, if $\Delta \in \left[0,\frac{\pi}{2}\right]$,