

Interface roughness scattering effect on electrical properties of heterojunctions

Scientific research paper

Zhaleh Ebrahiminejad^{1*}, Seyed Farhad Masoudi², Amir Hoshang Ramezani¹, Siamak Hosseinzadeh³, Somayeh Asgary¹

¹Department of Physics, West Tehran Branch, Islamic Azad University, Tehran, Iran

²Department of Physics, K.N. Toosi University of Technology, P.O. Box 15875-4416, Tehran, Iran

³Center for Asset Integrity Management, University of Pretoria, Pretoria, South Africa

ARTICLE INFO	ABSTRACT
Article history: Received 4 February 2022 Revised 7 March 2022 Accepted 28 March 2022 Available online 3 July 2022	In the present work, the effect of roughness in resonant tunneling diodes has been
	considered to track two main goals. At first, the roughness impact on the transport through
	these heterojunctions has been studied before investigating the roughness type effect. For
	calculating the electrical transport, the transfer matrix technique has been used in the
	simulations. Two different standard methods of deposition - Random deposition (RD),
Kenwords	and Ballistic deposition (BD)- have been applied to generate two dissimilar rough
Standard deposition method	interfaces. The scattering process reduces the transport probability. The conductivity as a
Transport	function of voltage has also been calculated. Effect of interface roughness on the peak-to-
Current density	valley current ratio in the presence of roughness has been discussed. The results show that
Roughness	the scattering effect it significant. As the applied voltage increases, at first, the value of
	current reaches its maximum amount, and then with increasing the voltage, the current
	falls in a negative differential resistance region.

1 Introduction

For many years the transport through resonant tunneling diodes (RTD) has been interested. The RTDs have been developed now for different applications such as high speed logic, high speed adders, analog-todigital conversion, and low power memory cells [1-3]. As all produced interfaces are rough, the RTD device designing requires to use the interfaces with desired properties. The transport properties and current density of these structures vary dramatically with interface roughness type [4, 5]. There are many various experimental and theoretical methods to generate rough thin films, for example solid on solid, random deposition with surface relaxation [6-10]. In RD model, particles are only allowed to stick on topmost of previous particles or on the substrate. As sideways sticking is not allowed, the columns grow independently. But, in the BD model, a particle falls down and sticks to the first particle or on the substrate. Therefore, the correlation occurs between columns laterally [11]. These growth methods have been selected based on the produced device applications. In the recent decades, the effect of growth method (and then the roughness type) has been studied on the RTDs. The results are dependent to the conditions of producing the surfaces/interfaces [12-15]. In the present work, it is interesting to study the different types of deposition models that produce the RTD interfaces. The first and third interfaces of the structure have been considered rough. These interfaces have been produced with BD and RD standard models, respectively. Indeed, the effect of two different rough interfaces could be studied simultaneously. The portion of scattered component of transmission as a function of incident electron energies have been calculated. The I-V characteristic and the PVR ratio are affected by roughness scattering. Also, the position of rough interfaces has been investigated on the transport properties.

2 Calculations and results

The RTDs for non-perfect interfaces, have a current density as a function of the bias voltage V written as [16]

$$j(V) = \frac{em^*k_BT}{4\pi^2\hbar^3} \times \int_0^\infty T(E, V) \times \ln\left[\frac{1 + \exp\left[\frac{(E_F - E)}{k_BT}\right]}{1 + \exp\left[\frac{(E_F - E - eV_{app})}{k_BT}\right]}dE, \quad (1)$$

Where, m* is the effective mass of the electron. $m_1=0.067m_0$ and $m_2=(0.067x+0.083x)$ are the effective masses associated to regions 1 and 2 respectively, while m_0 is the free electron mass [16]. T(E,V) is the transmission probability which is calculated by the envelope function Schrodinger equation and the continuity conditions of wave functions (the transfer matrix method). $V = \Delta E_c [\theta(z - \delta(r))]$ is the height of roughness, $\delta(r)$ expressions the interface height roughness, ΔE_c is the usual band offset amongst the adjust layers. It is 60% of $\Delta E_g = 1.15x + 0.37x^2$ (eV), where x is the aluminum content, $\theta(z)$ shows the unit step function. Here, the effect of interface roughness of the RTD contains of a GaAs/Al_xGa_{1-x}As double barrier structure that has been numerically studied. The values of the used parameters are as following. The barrier thicknesses and quantum well have been considered five nanometers. The details of calculations have been illustrated in Ref. [17].

Figure 1 shows the transmission probability vs energy of incident electrons and the aluminum content of x. The first and third rough interfaces of the structure have been produced based on two standard models BD and RD, respectively. Therefore, as the two interfaces of RTDs have been considered rough, the roughness has a main effect on the transmission probability. The portion of scattering increases and the transmission probability decreases compared to the structures perfect interfaces.



Figure 1. The transmission probability is calculated vs energy of incident electrons (ev) and aluminum content of x.

To illustrate the effect of roughness scattering, the scattered components of transmission probability vs energies of incident electrons have been shown in Figure 2 for two different values of x. The energy band gap ΔE_g of alloys depends on the aluminum content of x. The value of gap is direct and indirect for x smaller than $x_c = 0.45$ and x bigger than $x_c = 0.45$, respectively [16].

Based on Figures 2, the predominant effect of rough interfaces is obvious. In the perfect case, the maximum achievable resonance of transmission probability is unity. But, in the presence of roughness, this value decreases for RTDs for two different of x. The origin of the peaks and valleys of curves is as follows. The resonant tunneling happens when the energies of incident electrons match the wells lowest quasibound energy level.



Figure 2. The scattered portion of transmission is calculated vs energy of incident electrons (ev) and the aluminum content of x.

Because of roughness scattering, the resonances (constructive interference) and anti-resonances (destructive interference) appear. The anti-resonances are called "Fano" phenomena [18]. Moreover, these descriptions can illustrate the resonant peaks in the I-V characteristic. Figure 3 illustrates the current density vs bias voltage.



Figure 3. The current density vs the bias voltage and aluminum content of x.

The scattering portion of current density has been shown in Figure 4 to present clearly the interfacial roughness effect on electrical conductivity. It can be seen that as the aluminum content increases, the current density Logarithm vs bias voltage v decreases.



Figure 4. The portion of scattered current density as a function of the bias voltage and Aluminum content of x.

As it can be seen through the tunneling phenomena, the energy of electrons corresponds to a quasi-bound level in the central layer (well) and therefore a peak appears in the (I-V) characteristics. With increasing the V, at first, the current shows a maximum rate and then for higher values of V, a negative differential resistance region (NDR) appears. In other words, at high electric fields, one can see that with further continuous increase of the electric field, the decrease of current across the device can be achieved in some systems. Because of the shape of the I-V curve, the NDR phenomena can be classified into NDR (N-shaped). Due to interface roughness, as the scattering increases, the total transmission probability and current density decreases consequently. Also, the current valley increases and the PVR ratio of current is smaller than the perfect case. As a conclusion, the roughness scattering influences the current valley of RTDs. Therefore, there is disagreements between theoretical expectations and experiments works of PVR ratio [17-20]. The interfaceroughness effects on resonant tunneling process has been detected in RTDs with a greater difference of energy-gap amongst the barrier and well layers [16, 21]. Also, the results show that, the changing of interfacial roughness types of first and third interfaces does not have the perceptible effect on the results of the transport properties.

3 Remarks

The study of transport properties of resonant tunneling diodes with rough interfaces has been carried out. Because of rough interfaces, the scattering process results in transmission probability decrease. Also, the conductivity as a function of voltage has been calculated. The I-V characteristic has been investigated, the roughness scattering mechanism affects the current valley value of RTDs and it may describe the differences of theoretic predictions of PVR ratio bigger than experiments. Also, the numerical results do not show the difference consequences when the interfacial roughness types of rough first and third interfaces changed.

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