Nanostructured electrodes for thermo-tunnel and thermionic devices

Avto Tavkhelidze
Micro and Nano Electronics Research Institute, Tbilisi State University, Chavchavadze ave. 13, 0179 Tbilisi, Georgia

Abstract: *Low WF electrode, composed from a metal Ridged quantum well (RQW) layer and a base substrate, is proposed. The substrate material was selected so that electrons were confined to the RQW. The work function (WF) value depends on ridge geometry and electron confinement. We calculate WF in the metal RQW films grown both on a semiconductor and metal substrates. For most material pairs, the WF was reduced dramatically. Such structures, can serve as electrodes for thermionic and thermo-tunnel energy converters and coolers, operating at room temperatures.*

Keywords: nanostructuring; thermionic; thermo-tunnel

Introduction

Low work function (WF) electrodes [1] are essential for cold emission and room temperature operation of thermionic and thermo-tunnel [2] energy converters and coolers. Such electrodes require materials having work function as low as $e\phi = 0.2 - 0.4$ eV (here, e is electron charge and ϕ potential). It is extremely difficult to obtain such low WF values. To overcome difficulties, quantum mechanical tunnelling was utilized. Tunnelling through vacuum nanogap allows sufficiently large currents from the electrodes, having relatively high $e\phi$ values. However, vacuum nanogap device appears extremely difficult to fabricate [3-4] as it requires an electrode spacing of 5-10 nm. If an $e\phi$<1eV electrode could be obtained, thermionic and mixed regimes can be realized in wider vacuum gaps.

Here, we offer to reduce $e\phi$ using surface nanostructuring. The electrode is coated by the metal RQW layer. Its operation is based on the effect of quantum state depression. Periodic ridges, fabricated on the layer surface, impose additional boundary conditions on the electron wavefunction. Supplementary boundary conditions forbid some quantum states for free electron, and the quantum state density in the energy $\rho(E)$ reduces. According to Pauli's Exclusion Principle, electrons rejected from the forbidden quantum states, have to occupy the states with higher E. As result the Fermi energy E_F increases and $e\phi$ decreases [5]. The quantum state density in the RQW (figure 1) reduces G times

$$\rho(E) = \rho_0(E)/G \, , \qquad (1)$$

where $\rho_0(E)$ is the density of states in a conventional quantum well layer of thickness L (a = 0) and G is the geometry factor introduced in. In the first approximation, for the case $a << L, w$ and within the range $5 < G < 10$, the following simple expression can be used

$$G \approx L/a \, , \qquad (2)$$

where a is the ridge height and L is the RQW layer thickness (figure 1).

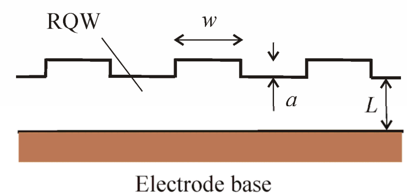

Figure 1. Cross section of electrode coated by RQW.

Density of forbidden quantum states is:

$$\rho_{FOR}(E) = \rho_0(E) - \rho_0(E)/G = \rho_0(E)(1 - G^{-1}) \qquad (3)$$

To determine the number of rejected electrons n_{REJ}, (3) should be integrated over the energy region in which the electrons are confined to the RQW.

$$\int_{CON} dE\, \rho_{FOR}(E) = (1 - G^{-1}) \int_{CON} dE\, \rho_0(E) = (1 - G^{-1})\, n_{CON} \qquad (4)$$

Here, $n_{CON} = \int_{CON} dE\, \rho_0(E)$ is the number of quantum states (per unit volume) within electron confinement energy region (which depends on substrate and RQW band structures and band offset). The RQW retains quantum properties at G times more width with respect to the conventional quantum well.

Work function of metal RQW grown on semiconductor substrate

To maintain the uniform vacuum nanogap over the whole area, electrodes should have plane geometry and smooth surface. The simplest solution is to use semiconductor substrate as an electrode base and grow a thin metal RQW layer on it. We consider the case when the difference between initial WF $e\phi_0$ and semiconductor electron affinity $e\chi$ was negative, i.e, $e(\phi_0 - \chi) < 0$ (fig. 2a). Here, electron confinement energy region is $\Delta E^{(0)}_{con} = E_g$. Electrons, rejected from the forbidden quantum states within $\Delta E^{(0)}_{con}$, occupy the empty states above $E^{(0)}_F$ and $e\phi$ reduces. As $e\phi$ reduced $e(\phi - \chi)$ also reduced and got even more negative.. Semiconductor bands curve in the direction of $E^{(m)}_C$. At the same time, ΔE_{con} width remains

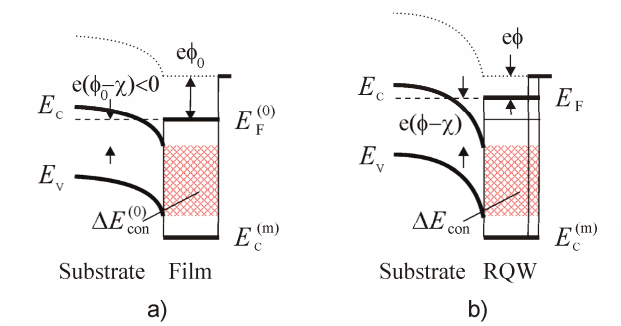

Figure 2. Energy diagram of metal-semiconductor contact for $e(\phi_0 - \chi) < 0$, a) without periodic ridges on the surface b) with ridges.

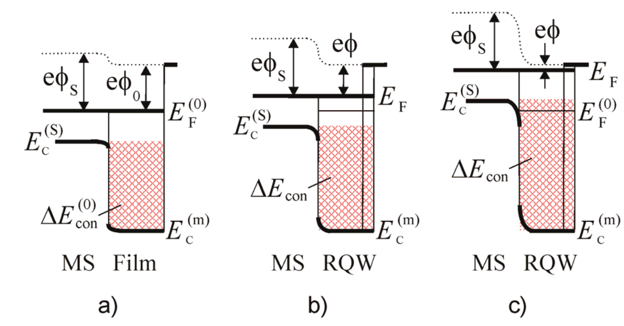

Figure 3. Energy diagram of metal-metal contact for the case $e\phi_S > e\phi_0$. a) Without periodic ridges, b), c) with ridges. MS depicts metal substrate.

constant. Electrons were rejected from the interval $e\chi_{\mathrm{m}} - e\chi - E_{\mathrm{g}} < E < e\chi_{\mathrm{m}} - e\chi$, and their number was calculated by applying this interval to (4). Electrons were injected in the interval $e\chi_{\mathrm{m}} - \phi_0 < E < e\chi_{\mathrm{m}} - e\phi$ and their number was $\int_{e\chi_m - e\phi_0}^{e\chi_m - e\phi} dE\,\rho_0(E)$ Using condition $n_{\mathrm{REJ}} = n_{\mathrm{INJ}}$, and $\rho_0(E) \propto E^{1/2}$, we found that

$$e\phi = e\chi_{\mathrm{m}} - \left\langle \left(e\chi_{\mathrm{m}} - e\phi_0\right)^{3/2} + \left(1 - G^{-1}\right)\varepsilon_1 \right\rangle^{2/3}. \quad (5)$$

Where $\varepsilon_1 = \left(e\chi_{\mathrm{m}} - e\chi\right)^{3/2} - \left(e\chi_m - e\chi - E_{\mathrm{g}}\right)^{3/2}$.

Work function of metal RQW grown on metal substrate

In the case of metal-RQW/metal contact, electrons are confined to the material having wider conduction band (fig. 3). Within $\Delta E_{\mathrm{con}}^{(0)}$, quantum states for electrons are filled in the metal film and forbidden in the metal substrate (MS). Let us begin from the case $e\phi_S > e\phi_0$, where $e\phi_S$ is the MS work function. Owing to WF difference, the contact potential emerges and the bottoms of conduction bands curve near the contact as shown in fig. 3a. When ridges are fabricated on the surface (fig. 3b, 3c), some electrons are rejected from $\Delta E_{\mathrm{con}}^{(0)}$ and injected above $E_{\mathrm{F}}^{(0)}$. Fermi level moves up on energy scale. The $E_{\mathrm{C}}^{(\mathrm{S})}$ follows the Fermi level (fig. 4b). The electron confinement energy region $\Delta E_{con} = E_{\mathrm{C}}^{(\mathrm{S})} - E_{\mathrm{C}}^{(\mathrm{m})}$ increases. This leads to rejection of even more electrons and $e\phi$ reduction amplifies. However, with rising E_{F}, number of states $\int dE\,\rho_0(E) \propto E^{3/2}$ above E_{F} increase more rapidly than n_{REJ} (as $E_{\mathrm{F}} > E_{\mathrm{C}}^{(\mathrm{S})}$) and at some $e\phi$ value, equilibrium is maintained.

Analysis conducted on the basis of electron number conservation in conduction band [6] shows that $e\phi$ is calculated using equation

$$\left(1 - G^{-1}\right)\left(e\chi_{\mathrm{m}} - e\phi + e\phi_S - e\chi_S\right)^{3/2} = \left(e\chi_{\mathrm{m}} - e\phi\right)^{3/2} - \left(e\chi_{\mathrm{m}} - e\phi_0\right)^{3/2}. \quad (6)$$

When using semiconductor substrate, wide band gap material allows more electron confinement and lower values of resulting $e\phi$. Dependence of $e\phi$ on the band gap was analyzed for a number of cases and the corresponding formulae derived. When using metal substrate, materials with low Fermi energy allow more electron confinement and lower values of resulting $e\phi$.

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