## A Multi-Subband Design Theory for a

## **Terahertz-Frequency Double-Barrier Quantum-Well Oscillator**

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## ABSTRACT

This paper presents a theory of the creation of current oscillation in a multisubband system. The oscillation in the system originates from the intersubband coupling. The relationship between the oscillation frequency and the subband structure can be used as a design criterion for a new class of intrinsic oscillators.

The search for compact solid-state, highfrequency power sources has been an important research subject for many years. Since the end of 1980's, resonant tunneling diodes (RTD) have been treated as a possible high frequency power sources. However, as it is well known, the traditional implementation of a RTD has not been successful as a source at terahertz (THz) power frequency. This failing is due to the extrinsic design manner of the oscillator that utilizes external circuit elements to induce the oscillation. In contrast to the extrinsic design of RTD oscillators, the intrinsic design of RTD oscillators makes use of the microscope instability of RTDs directly. This type of an approach will avoid the drawbacks associated with the extrinsic implementation of RTD's. It is believed that if the dynamics surrounding the intrinsic oscillation can be understood and controlled, RTD sources based on the self-oscillation process should yield milliwatt levels of power in the THz regime. However, the exact origin of the high-frequency intrinsic current oscillation has not yet been fully established. The lack of knowledge related to the origin of the intrinsic instabilities in double-barrier quantumwell structures (DBQWSs) directly hampers realizing an optimal design (device and circuit) of a RTD-based oscillator. Thus, it is extremely important to understand the creation mechanism of the intrinsic instability in DBQWSs.

Previously, a new theory was presented by our group that provided a basic idea for the origin of the intrinsic oscillation in a DBQWSs [1]. This theory revealed that the current oscillation, hysteresis and plateau-like structure in I-V curve are closely related to the quantum mechanical wave/particle duality nature of the electrons. In addition, these effects were shown to be a direct consequence of the development and evolution of a dynamical emitter quantum well (EQW), and the ensuing coupling of the quasidiscrete energy levels that are shared between the EQW and the main quantum-well (MQW) formed by the DBQWS. This paper will extend the earlier theory through the application of basic quantum mechanical model. A multi-subband model for the describing the electron dynamics in DBQWSs is given. The multi-subband based theory will provide a simple relationship

between the oscillation frequency and the energy-level structure of the system.

Our previous research showed that a DBQWS becomes a multi-subband system once the emitter quantum well (EQW) is crested. For a multi-subband system, the wavefunctions of the system can be written as

$$\psi(z,t) = \sum_{k=1}^{n} \psi_k(z,t) e^{-\frac{2\pi i}{h} F_k(t)}$$
(1)

where

$$F_{k}(t) = \int_{0}^{t} dt' E_{k}(t)$$
 (2)

In terms of the fundamental definitions of current and density, the density and current can be expressed as

$$j(t) = \sum_{k} \langle \psi_{k} | \hat{j} | \psi_{k} \rangle + 2 \operatorname{Re} \sum_{k,l(l < k)} \langle \psi_{k} | \hat{j} | \psi_{l} \rangle e^{-2\pi \frac{F_{l}(t) - F_{k}(t)}{h}}$$
$$\rho(t) = \sum_{k} \psi_{k}^{*} \psi_{k} + 2 \operatorname{Re} \sum_{k,l(l < k)} \psi_{k}^{*} \psi_{l} e^{-2\pi \frac{F_{l}(t) - F_{k}(t)}{h}}$$

Generally speaking, these two formulas show that there are no oscillations in a multi-subband system. However, if a system meets the following criteria, the oscillations do exist in the system.

Energy criteria: There are three conditions regarding to the relationship between the subband energies. If current oscillations exist in a multi-subband system, one of the conditions has to be satisfied. The following are the conditions.

1. Maximum Subband Coherence: The energy differences between the subbands are equivalent, that is,

 $\Delta E(t) = \Delta E_{lk}(t) = |E_l(t) - E_k(t)| = const$ Here,  $l \in \{l_i\}, k \in \{k_j\}$ , and l < k. The sets  $\{l_i\}$  and  $\{k_j\}$  are of equal number and assume all possible values from the number sequences  $1, 2, \dots, n$ .

2. Partial Subband Coherence: A finite and countable number of energy differences are equivalent, that is,  $\Delta E(t) = \Delta E_{lk}(t) = |E_l(t) - E_k(t)| = const$ Here,  $l \in \{l_i\}, k \in \{k_j\}$ , and l < k. The sets  $\{l_i\}$  and  $\{k_j\}$  are of equal number and assume some of the values from the number sequences  $1, 2, \dots, n$ .

3. Minimum Subband Coherence. The intrinsic oscillation is characterized by the condition in which only a single set of subbands contributes to the instability, that is,

 $\Delta E(t) = \Delta E_{lk}(t) = |E_l(t) - E_k(t)| = const$ where *l* and *k* can assume only one set of values from the energy level index 1,2,...,*n* and *l* < *k*.

Wavefunction criterion: The wavefunctions of the energy levels that cause the oscillation should be spatial overlapped. That is  $\psi_i \psi_j \neq 0$  if the *ith* and the *jth* energy levels are able to cause the oscillation.

If the energy criteria and the wavefunction criterion can be satisfied simultaneously, the current and density can be expressed as

$$j(t) = \sum_{k} \langle \psi_{k} | \hat{j} | \psi_{k} \rangle + 2 \operatorname{Re} \left\{ e^{-2\pi \frac{\Delta F(t)}{h} - i\alpha(t)} \mathcal{Q}(z, t) \right\}$$
$$\rho(t) = \sum_{k} \psi_{k}^{*} \psi_{k} + 2 \operatorname{Re} \left\{ e^{-2\pi \frac{\Delta F(t)}{h} - i\beta(t)} H(z, t) \right\}$$

where  $\Delta F(t) = \int_{0}^{t} dt' \Delta E(t')$  and  $\alpha$  and  $\beta$  are periodical functions of time.

Obviously, these formulas show that *the intrinsic current oscillation in a multisubband system originates from the intersubband coupling*. The previous derivations lead to a simple relation,  $v = \Delta E_0/h$  for defining the oscillation frequency This relationship can be regarded as the basic design formula for the oscillator.

In order to verify our theory, a selftime-dependent consistent, Wigner-Poisson numerical investigation has been reveal sustained current used to oscillations in an isolated DBOWSbased device. The structure of the device has been described elsewhere [1]. The potential profiles obtained are then used in a Schroedinger-based approach to derive the energy level structure and the associated wavefunctions as shown in Figs. 1 and 2. From Fig. 1, we can see that only  $E_2$  and  $E_3$  contribute to the oscillation since the wavefunctions of these states are located in the same spatial region. Calculations show there is only 1% difference between the frequency from the Wigner-Poisson simulation and that from the formula  $v = \Delta E_0 / h$ .



**Figure 1.** The quantum subband structure that is used to reveal the underlying source of the oscillations.



Figure 2. The wavefunctions of the subbands in the system.

Insight into DBQWSs as potential devices for high-frequency very oscillators is facilitated through two Together, these simulation studies. studies establish the fundamental principals and basic design criterions for the future development and implementation DBQW-based of oscillators. Further, this paper provides physical interpretations of the instability mechanisms and explicit guidance for defining new structures that will admit enhanced oscillation characteristics. Also, the theory has been used to probe the possible device structures that can create oscillations in the positive differential resistance region of the average I-V curve. These physics-based models and design criteria will be used in the future to facilitate the design of a realistic oscillator where a tunneling structure is integrated and optimized within an embedding circuit.

## References

[1] Peiji Zhao, H. L. Cui and D. Woolard, Physical Review B63, 75302(2001); Peiji Zhao, D. Woolard, and H. L. Cui, Phys. Rev. B67, 085312(2003). argon atmosphere. The background pressure in a vacuum chamber prior to deposition was about  $3 \times 10^{-7}$  mbar. The argon working pressure was  $6 \times 10^{-3}$  mbar and  $9 \times 10^{-3}$  mbar during Mo and Cu deposition correspondingly. The deposition rate was 1.7 nm/sec for Mo and 0.9 nm/sec for Cu. The calibration has been done independently using specially deposited films measured by alpha step profilometer. Finally samples were cut into pieces of  $24 \times 1.5$  mm<sup>2</sup> size to provide measurements.

Samples with the following Mo/Cu thickness values (nm) have been fabricated:

(1) 8/0, 8/30, 8/50, 8/100;
(2) 12/0, 12/30, 12/50, 12/100;
(3) 15/50, 25/50, 35/50, 50/50;
(4) 10/40, 15/35, 20/30, 30/20.

Dependencies of resistance versus temperature R(T) have been measured in <sup>3</sup>He/<sup>4</sup>He dilution refrigerator using four-probe method. The transition edge temperature of samples with Mo thickness 12 – 15 nm turned out to be the most sensitive to Cu thickness. Such samples have shown the transition edge temperature in the range  $\approx 0.075 - 0.4$  K, which is required for bolometer operation. Samples with thinner Mo layer haven't demonstrated the superconducting transition at all. R(T) dependencies for Mo/Cu thickness values 15/35 and 12/100 (nm/nm) are shown on Fig.1 together with R(T) dependence for pure Mo film of 12 nm thickness.

The effect of proximity is clearly seen from the Fig.1. The transition edge temperature decreases with thickening of the Cu layer, simultaneously the resistance of bi-layer structure getting smaller. The pure Mo film has shown transition temperature of  $\approx 0.93$  K, which is expected value for Mo.

The parameter  $\alpha = T / R \cdot dR / dT$ , which characterizes the abruptness of superconducting transition, has been estimated in the vicinity of the superconducting transition edge temperature  $(T_c)$  for three measured samples. It was found to be  $\alpha \approx 1070$  for  $T_c \approx 0.93$  K,  $\alpha \approx 150$  for  $T_c \approx 0.4$  K and  $\alpha \approx 510$  for  $T_c \approx 0.08$  K. This parameter determines the speed response: the larger  $\alpha$  the smaller response time of bolometer [3]. The value of  $\alpha$  found in our measurements for  $T_c \approx 0.08$  K and 0.4 K is about two times smaller in comparison with this value reported in [3] for similar bi-layer structure. Probably it can be explained by nonuniformity of our sputtered thin films.

Obtained results will provide the basis for subsequent developments of bolometer microcircuits with transition edge sensor of micrometer and sub-micrometer size.

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