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THEORETICAL MODEL FOR NEGATIVE DIFFERENTIAL CONDUCTANCE IN 2D SEMICONDUCTOR MONOLAYERS

A simple theoretical model of electron heating in a system with two valleys is applied for the first time to describe 2D semiconductor monolayers of the MoS_2 and WS_2 types. The model is demonstrated to describe sufficiently well the available experimental data on the negative differential conductance effect in a WS_2 monolayer. It confirms a possibility to fabricate Gunn diodes of a new generation based on the structures concerned. Such diodes are capable of generating frequencies of an order of 10 GHz and higher, which makes them attractive for many practical applications.

Keywords: differential conductance, semiconductor monolayers of the MoS_2 and WS_2 types.

A carbon atomic monolayer, graphene, was obtained for the first time in 2004. It was found to be semimetal [1]. Therefore, its parameters can hardly be used to implement essentially different states "0" and "1", which became a principal obstacle on the way to the creation of the graphene-based hardware components for new electronics. Numerous attempts to induce semiconductor-like properties in graphene (by the hydrogenation, creation of nanostripes, inserting defects, and so forth; see work [2] and references therein) turned out unsuccessful from the viewpoint of further practical applications.

However, during last years, other monolayers with semiconducting properties (MoS_2, WSe_2, and other chalcogenides of transition metals, black phosphorus, and others; see, e.g., works [3,4]) were intensively synthesized and studied. The most known from this class of materials are the MoS_2 and WS_2 monolayers. They are direct-band semiconductors with the band gap widths $E_g \approx 1.7$ and 1.8 eV, respectively. The extrema of the conduction and valence bands are located at points K and K' of the hexagonal Brillouin zone [5], as it takes place in graphene.

The results of calculations carried out from the first principles, by using the density functional method demonstrated that the conduction band spectrum of those materials includes a lateral extremum (the T-valley) with energies by approximately 0.2 and 0.08 eV larger than the band bottom energy, which is located in the direction from the points K and K' to the Brillouin zone center Γ (Fig. 1). The energy spectrum near those two extrema is parabolic. The presence of two subbands in the conduction band – lower (denoted by subscript 1) and upper (denoted by subscript 2) ones, for which the effective-mass relation $m_1 < m_2$ for two-dimensional electrons is obeyed [5] – gives us grounds to expect that the effect of negative differential conductance, which is associated with the filling by field-heated electrons of the higher val-

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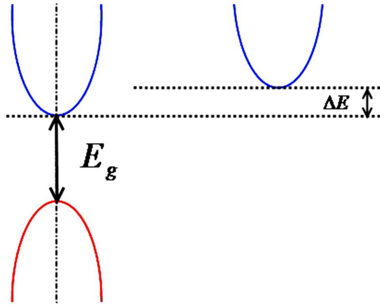

Fig. 1. Structure of the conduction band in monolayers of transition metal chalcogenides. The presence of K- and T-valleys allows the effect of negative differential conductance

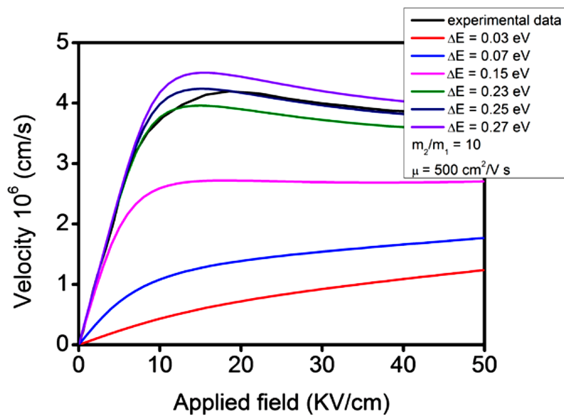

Fig. 2. Dependences of the drift velocity in WS_2 on the applied field calculated according to Eq. (4) for the temperature $T = 300$ K and various ΔE-values. The solid curve is the corresponding experimental dependence according to the results of work [10]

ley characterized by a higher effective mass, can take place in 2D monolayers of the WS_2 or MoS_2 type [6]. Note that this effect has already been observed in "traditional" quantum heterostructures [7]. Recently, it has been studied in quantum heterostructures composed of multilayered phosphorus and rhenium disulfide [8] or graphene (ultrathin graphite) and boron nitride [9].

Finally, the negative differential conductance has been experimentally revealed quite recently in WS_2 monolayers [10]. It was shown that if the monolayer is unstrained, the effect does not take place owing to a small energy distance between the valleys, $\Delta E \approx 0.08$ eV, because, at room temperature, electrons begin to fill the T-valley at minimum values of the fields between the gate and the drain. However, if a biaxial compression is applied, and $\Delta E \sim 0.1$ eV or somewhat larger, the effect of negative differential conductance begins to be clearly distinguished in the dependence of the current through the field transistor on the field between the gate and the drain.

The detected effect can open promising prospects for the creation of microwave devices in the frequency range of tens of gigahertz or higher. Therefore, it is important to have a convenient semiphenomenological model for its description, similar to that widely used for three-dimensional materials [6].

For the field-heated electrons redistributed between the valleys K (subscript 1) and T (subscript 2), the current density through the semiconductor can be written as follows:

$$J = e(\mu_1 n_1 + \mu_2 n_2)\varepsilon = env, \qquad (1)$$

where the electron concentrations $n_{1,2}$ in two subbands are related by the equality $n_1 + n_2 = n$, ε is the electric field strength, and v the average drift velocity of electrons. The electron concentration ratio between the subbands is associated with the energy ΔE and the temperature of hot electrons T_e by the obvious expression [6]

$$\frac{n_2}{n_1} = R\,\exp\left(-\frac{\Delta E}{kT_e}\right), \qquad (2)$$

where the factor R is the ratio between the numbers of available quantum states in subbands 2 and 1. Taking into account that the degeneration degree equals $g_1 = 2$ in the K-valley, and $g_2 = 6$ in the T-valley [5], and adopting standard expressions for the 2D densities of state in the case of parabolic spectrum, $D_{2D} = \frac{g_{1,2} m_{1,2}}{\pi\hbar^2}$, we obtain

$$R = 3\frac{m_2}{m_1} \gg 1. \qquad (3)$$

In the approximation of the energy relaxation time τ_e, the dependence of the drift velocity on the field can be written in the standard form

$$v = \mu_1 \varepsilon \left[1 + \frac{n_2}{n_1}\right]^{-1}. \qquad (4)$$

The electron temperature T_e that enters Eqs. (2) and (4) looks like

$$T_e = T + \frac{3e\tau_e\mu_1}{3k}\varepsilon^2 \left[1 + \frac{n_2}{n_1}\right]^{-1}. \qquad (5)$$

Figure 2 demonstrates the dependences of the electron drift velocity (4) in WS_2 on the applied field calculated according to Eqs. (2), (3), and (5) for the temperature $T = 300$ K and various ΔE-values from 0.03 to 0.27 eV. Figure 3 exhibits the dependences of the ratio between the electron concentration n_2 in the upper T-valley and the total electron concentration n in the conduction band on the electric field ε calculated for the same room temperature.

In the calculations, the following parameter values were used: $\tau_e = 10^{-12}$ s, $\mu_1 = 500$ cm^2/(V s), $m_2/m_1 = 10$. At $\Delta E = 0.25$ eV, the indicated values provide a good agreement with the experimental curve and correlate with the data given for WS_2 in the literature (see work [10]). Note that the ratio between the effective masses in the K- and T-valleys (in accordance with the data presented in work [9], this parameter equals $0.32m_0$ and $0.75m_0$, respectively) is somewhat lower, but the given values are relevant only in vicinities of the extrema and do not make allowance for the mass increase with the energy in the T-valley.

One can see from Fig. 2 that, starting from a certain threshold value $\Delta E \approx 0.15$ eV, the dependence $v(\varepsilon)$ acquires a maximum, and the ratio n_2/n begins to grow at the fields corresponding to this maximum (this phenomenon corresponds to the intensive filling of the upper valley in the conduction band by heated electrons), which also qualitatively corresponds to the results of work [10]. At lower ΔE-values, as is shown in Fig. 3, electrons actively transit to the upper valley already at the minimum electric field values ε, and the effect of negative differential conductance is absent.

Hence, a simple theoretical model of electron heating in a system with two valleys [6], which was adapted by us for the first time to describe 2D semiconductor monolayers of the MoS_2 and WS_2 types, can well describe available experimental data. It confirms the possibility to create a new generation of Gunn diodes on the basis of those structures. The frequencies that can be obtained with such diodes can be easily estimated from the relation

$$f \sim \frac{v}{L}, \qquad (6)$$

where L is the diode channel length. For the parameter values corresponding to the system that was studied in work [10] ($v = 4 \times 10^6$ cm/s and $L = 5$ μm),

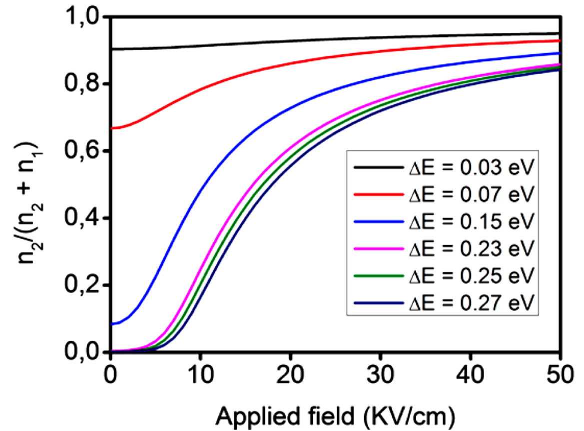

Fig. 3. Dependences of the ratio between the electron concentration in the upper T-valley, n_2, and the total electron concentration in the conduction band, n, on the electric field ε calculated for $T = 300$ K

we obtain $f \sim 10$ GHz, which makes such diodes potentially attractive for a number of practical applications.

The model described in this paper also makes it possible to estimate a potential capability to create Gunn diodes on the basis of other 2D semiconductor monolayers and thin quantum wells, which are based on both traditional electronic materials and carbon allotropes "between graphene and graphite". The latter, as we showed in work [11], can also possess useful semiconductor properties.

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ТЕОРЕТИЧНА МОДЕЛЬ ДЛЯ ЕФЕКТУ НЕГАТИВНОЇ ДИФЕРЕНЦІАЛЬНОЇ ПРОВІДНОСТІ У 2D НАПІВПРОВІДНИКОВИХ МОНОШАРАХ

Р е з ю м е

Нами вперше адаптовано для 2D напівпровідникових моношарів типу MoS_2 та WS_2 просту теоретичну модель розігріву електронів у системі з двома долинами. Показано, що така модель добре описує наявні експериментальні дані щодо ефекту негативної диференціальної провідності в моношарі WS_2 й підтверджує можливість створення на таких структурах нового покоління діодів Ганна. Частоти, які може бути отримано на таких діодах, становлять порядку 10 ГГц і вище, що робить такі діоди потенційно привабливими для низки практичних застосувань.