- [7] Kresse, G., Furthmüller. Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set. Computational materials science, 6(1), 15-50 (1996).
- [8] Chaput, L., Togo, A., Tanaka, I., Hug, G. Phonon-phonon interactions in transition metals. Physical Review B, 84(9), 094302 (2011).
- [9] Togo, A., Tanaka, I. First principles phonon calculations in materials science. Scripta Materialia, 108, 1-5 (2015).
- [10] Togo, A., Chaput, L., Tanaka, I. Distributions of phonon lifetimes in Brillouin zones. Physical Review B, 91(9), 094306 (2015).
- [11] Tamura, S. I. Isotope scattering of dispersive phonons in Ge. Physical Review B, 27(2), 858-866 (1983).
- [12] Molina-Sanchez, A., Wirtz, L. Phonons in single-layer and few-layer MoS2 and WS2. Physical Review B, 84(15), 155413 (2011).
- [13] Ataca, C., Topsakal, M., Akturk, E., Ciraci, S. A comparative study of lattice dynamics of three-and twodimensional MoS2. The Journal of Physical Chemistry C, 115(33), 16354-16361 (2011).
- [14] Kan, M., Nam, H. G., Lee, Y. H., Sun, Q. Phase stability and Raman vibration of the molybdenum ditelluride (MoTe2) monolayer. Physical Chemistry Chemical Physics, 17(22), 14866-14871 (2015).
- [15] Guo, H., Yang, T., Yamamoto, M., Zhou, L., Ishikawa, R., Ueno, K., Saito, R. Double resonance Raman modes in monolayer and few-layer MoTe2. Physical Review B, 91(20), 205415 (2015).
- [16] Li, W., Carrete, J., Mingo, N. Thermal conductivity and phonon linewidths of monolayer MoS2 from first principles. Applied Physics Letters, 103(25), 253103 (2013).
- [17] Gu, X., Yang, R. Phonon transport in single-layer transition metal dichalcogenides: A first-principles study. Applied Physics Letters, 105(13), 131903 (2014).

GATE LEAKAGE CURRENT IN AIGaN SCHOTTKY DIODE IN TERMS OF PHONON-ASSISTED TUNNELING MODEL

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I. INTRODUCTION

AlGaN/GaN high electron mobility transistor (HEMT) has long been regarded as an excellent candidate for power devices with low power consumption. However, performance of Schottky-gated HEMT is strongly limited by an excessive gate leakage current. Suppositions of researchers about the reverse-bias leakage current in a Schottky contact are radically different, which implies that fundamental properties of the conduction mechanisms have not yet fully understood. Nevertheless, a comparative analysis of current-voltage characteristics of GaN Schottky diodes shows that the leakage current can be estimated in terms of a phonon-assisted tunneling (PhAT) model [1]. Although it was developed specifically for GaN, the model can be naturally assumed to remain valid for AlGaN, thus allowing calculating the leakage current in Schottky-gated HEMT.

II. SIMULATION DETAILS AND RESULTS

In this work, a two-dimensional vertical $Al_{0.3}Ga_{0.7}N$ Schottky diode structure is simulated in the framework of the thermionic emission-diffusion theory developed by Crowell and Sze [2] and expanded by the PhAT model. The structure consists of a 0.2 μ m high n-type doped semiconductor layer with the upper boundary to be a Schottky contact, while the lower boundary is Ohmic.

According to the PhAT model, the charge transport through the Schottky barrier is controlled by electron tunneling from states/traps located near the semiconductor-metal interface to the conduction band of the semiconductor. Due to continuous filling of the centers from the adjacent metal, the electron occupation of these states is assumed to be independent of the bias voltage. If the electrons emitted from the states dominate the charge flux through the barrier, the current density J is calculated as follows:

$$J = q\mu \left(\frac{n_{pip}}{1-\beta} + \frac{n_{eq}}{1-\frac{1}{\beta}}\right) E,$$
⁽¹⁾

where q is the elementary charge, μ is the electron mobility, neq is the equilibrium electron concentration and E is the electric field.

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The value of npip is given by

$$n_{pip} = -\frac{PN_s}{\mu E},\tag{2}$$

where P is the PhAT rate and Ns is the density of states occupied by electrons.

The value of β is given by

$$\beta = \frac{v_r}{\mu E'},\tag{3}$$

where v_r is the thermionic emission velocity of electrons.

The PhAT rate P as a function of the temperature T and the electric field E is defined as follows:

$$P(T,E) = \frac{-qE}{(8m^*E_t)^{\frac{1}{2}}} \Big[(1+\gamma^2)^{\frac{1}{2}} - \gamma \Big]^{\frac{1}{2}} [1+\gamma^2]^{-\frac{1}{4}} \times \\ \times \exp\left\{ \frac{4(2m^*)^{\frac{1}{2}}}{3q\hbar E} E_t^{\frac{3}{2}} [(1+\gamma^2)^{1/2} - \gamma]^2 \Big[(1+\gamma^2)^{\frac{1}{2}} + \frac{\gamma}{2} \Big] \right\},$$

$$(4)$$

where m^* is the electron effective mass, Et is the trap depth, \hbar is the reduced Planck constant and

$$\gamma = -\frac{(2m^*)^{\frac{1}{2}}\Gamma^2}{8q\hbar E E_t^{\frac{1}{2}}}.$$
(5)

In equation 5, Γ^2 is the width of the center absorption band and given by

$$\Gamma^2 = 8a(\hbar\omega)^2 (2b+1),$$
(6)

where a is the electron-phonon interaction constant, $\hbar\omega$ is the phonon energy and

$$b = \frac{1}{\exp\left(\frac{\hbar\omega}{\kappa T}\right) - 1},\tag{7}$$

where κ is the Boltzmann constant.

When employing these equations, the leakage current of the AlGaN Schottky diode is calculated to be equal $1.566 \cdot 10^{-9}$ A/µm at the anode voltage of -10 V. The results are consistent with the experimental data provided in [3].

III. CONCLUSIONS

The leakage current of the reverse-biased AlGaN Schottky diode can be described well in terms of the PhAT model.

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REFERENCES

- [1] P. Pipinys and V. Lapeika, "Temperature dependence of reverse-bias leakage current in GaN Schottky diodes as a consequence of phonon-assisted tunneling," J. Appl. Phys., vol. 99, 093709, 2006.
- [2] C. R. Crowell and S. M. Sze, "Current transport in metal-semiconductor barriers," Solid-St. Electron., vol. 9, pp. 1035-1048, 1966.

[3] M. Mi, Y. He, B. Hou, M. Zhang, J. Zhang, C. Wang, X. Ma and Y. Hao, "Threshold voltage engineering in GaN-based HEMT by using La2O3 gate dielectric," Phys. Status Solidi C, vol. 13, 325-327, 2016.

SIMULATION OF THE OPTICAL WAVES INTERACTION WITH NANOSTRUCTURE THIN ALUMINUM-NICKEL FILMS

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I. INTRODUCTION

Nanomaterials are widely used in different branches of science and technology – optics, power engineering, photoelectrochemistry, electronics, medicine and others. Thin films of nanometer sizes are used in luminescent materials, in solar batteries, in colorants with special properties, in mini sensors for adsorption of gases, in gas sensors, in explosives, etc. [1].

Thin films can be obtained by physical and chemical methods. The most popular of these are vacuum deposition, ion-beam sputtering, sol-gel method, thermal evaporation, chemical vapor deposition, spray pyrolysis of aerosols. The last noted method is one of the simple and economical. It is important that when thin films are obtained by pyrolysis, light alloying of any element in the corresponding fractions is ensured. This method is convenient to use when it is necessary to produce a homogeneous surface of thin films of highly required thickness and fully dense material [2].

The method of aerosol pyrolysis spray can be used for metal oxides, semiconductor oxides, superconducting thin films, binary and triple chalcogenides. The deposition velocity, the substrate temperature, the air pressure, the distance between the nozzles and the template are the main parameters that can be varied in this method. The ideal condition for the preparation of a film is the case when the droplets are completely removed from the solvent. In [3] the mathematical model of evaporation of micro- and nanosized drops is given, which allows to determine whether the particles will be filled or hollow.

Thin films, which represent a two-component structure of the absorber-reflector type, are at present the most common. Aluminum is a good absorber (absorption coefficient is more than 0.7, and the reflection coefficient is less than 0.3) in the ultraviolet range of wavelengths. The coefficient of reflection of nickel in this range is higher [4]. Therefore, the investigation of the optical properties of the aluminum-nickel nanomaterial is a priority.

II. EXPERIMENTAL METHOD

Different numerical methods allow analyzing the interaction of electromagnetic waves with nanoparticles. Classification of methods of wave modeling, as a rule, is carried out depending on their method of solution. The most known are the following methods: 1) finite differences in the time interval (FDTD), 2) finite elements (FE), 3) final integration (FIT), 4) moments (MoM), 5) integral equations.



Figure 1 – Graphical interpretation of the finite iteration method (FIT)

Software for solving such problems in the optical range is developed by the following companies: Rsoft's FullWaVE, Optiwave's OptiFDTD, EM Explorer Studio, EM Photonics FastFDTD, COMSOL