LATTICE THERMAL CONDUCTIVITY OF TRANSITION METAL DICHALCOGENIDES

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I. INTRODICTION

The monomolecular layers (MLs) of transition metal dichalcogenides (TMDs) are two-dimensional graphene-like materials which have great perspectives in electronics and optoelectronics due to the fact that they are direct-gap semiconductors with relevant band gap [1]. Moreover, monolayer TMDs have perspectives in spintronics and valleytronics [2]. An individual ML of TMDs can easily be synthesized from bulk TMDs [3] because bulk TMD is a layered crystal with weak interlayer Van der Waals bonds and strong intralayer forces. Also, they can be fabricated by means of bottom-up method like a chemical vapor deposition [4].

In most stable H-phase [5] one ML has trilayer sandwich structure Chal–Me–Chal (Chal = S, Se, Te; Me = Mo, W) with space symmetry of $P\bar{6}m2$ (№ 187). Within this H-phase the metal atom is located in a trigonal prism formed by the chalcogen atoms.

In recent years, a lot of attention is paid to exploration of these materials. In this work, we deal with phonon properties, in particular we carried out the ab initio investigation of lattice thermal conductivities. These properties are very important for the applications in integrated circuits or thermoelectric devices.

II. COMPUTATIONAL METHOD

The lattices optimization and calculations of harmonic and cubic anharmonic force constants (FCs) were performed by density functional theory (DFT) [6] within local density approximation (LDA) [6] by using Vienna Ab initio Simulation Package (VASP) [7]. The cutoff energy in all simulations was set to 320 eV.

The unit cell of monolayer TMD is the hexagonal cell with three atoms (one metal and two chalcogen atoms) and additional vacuum layer between MLs. In our work, thickness of this vacuum layer was chosen to be 12 Å.

For FCs calculations, the finite displacement method was applied [8]. We used 4×4×1 supercell and 6×6×1 k-mesh sampling for harmonic FCs calculations and 2×2×1 supercell and 12×12×1 k-mesh sampling for anharmonic cubic FCs calculations. Harmonic FCs were used for dynamic matrix creation within the phonopy package [9] for the calculations of phonon spectra and density of phonon states. Anharmonic cubic FCs were used for calculations of phonon relaxation time within the phono3py package by technique described in [10]. For boundary scattering, we used a very simple model provided by phono3py package [10]. Isotope scattering is described by the second-order perturbation theory [11]. All these results were used within the single mode relaxation time approximation (SMRTA) for the lattice thermal conductivity calculations [10].

III. RESULTS AND DISCUSSION

The calculated phonon spectra of monolayer TMDs have a good agreement with previous results [12–15]. The calculated xx- and yy-components of lattice thermal conductivity tensor of monolayer TMDs are equal to each other. Other calculated components of tensor are equal to zero. In this article, we assign by κ an xx-component of lattice thermal conductivity tensor.

Figure 1 shows the dependencies of κ on monolayer size L at room temperature for monolayer TMDs. Figure 2 shows the κ dependencies on temperature T with 1 μm monolayer size.

The calculated lattice thermal conductivities of monolayer TMDs have an agreement with previous results [16–17]. Diselenides and ditellurides of different transition metals are very similar, because these crystals have a very similar phonon spectra except highest phonon modes which are not important for κ value.

The monolayer WS_2 has noticeably larger value of κ than the monolayer MoS_2. It can be explained by the larger value of the gap between acoustic and optical modes $\Delta\omega$. The most possible phonon scattering processes is an interaction between two acoustic and one optical phonons. The monolayer WS_2 has a gap value $\Delta\omega$ fairly close to the frequency of the top of acoustic modes. This fact forbids a lot of scattering process because of the energy conservation law.

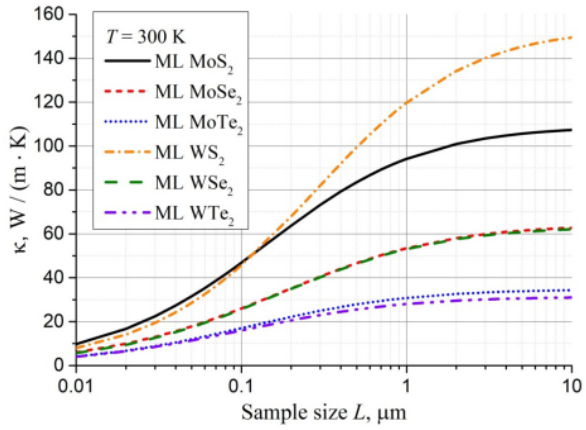

Figure 1 – The dependencies of lattice thermal conductivity κ on monolayer size L at room temperature for monolayer TMDs

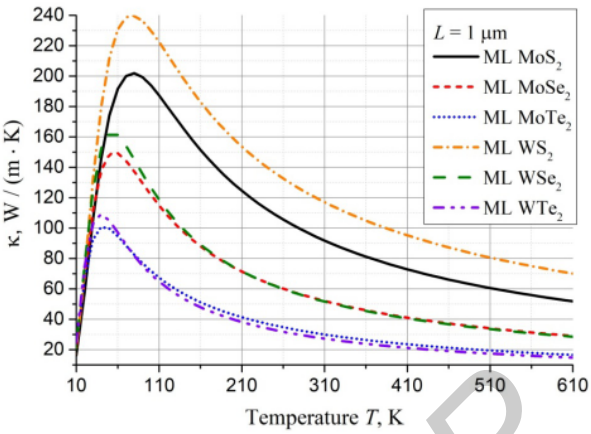

Figure 2 – The dependencies of lattice thermal conductivity κ on temperature T for monolayer size of 1 μm for monolayer TMDs

The calculated values of κ at room temperature with the monolayer size of 1 μm, the calculated values of gaps Δω and the calculated frequencies of the tops of acoustic modes for monolayer TMDs are presented in the Table 1.

Table 1 – Calculated κ at room temperature with the monolayer size of 1 μm, gaps Δω and frequency of the tops of acoustic modes of monolayer TMDs

	ML MoS_2	ML $MoSe_2$	ML $MoTe_2$	ML WS_2	ML WSe_2	ML WTe_2
κ, W / (m·K)	94.21	53.46	30.79	119.78	53.07	28.06
Δω, cm^{-1}	49.44	8.84	2.14	112.40	33.6	17.65
Top of acoustic modes, cm^{-1}	230.80	161.43	117.39	186.19	141.90	105.74

IV. CONCLUSION

The results of ab initio calculations of lattice thermal conductivities of monolayer transition metal dichalcogenides are analyzed and presented. The calculated values of lattice thermal conductivities are close to values of commonly used microelectronics materials (Si, Ge, GaAs).

The results of analysis can be used for better understanding of phonon transport mechanisms and for searching for new materials and ways of modifications of their properties.

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GATE LEAKAGE CURRENT IN AlGaN 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 μm 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:

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

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