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Electric charge transfer in molybdenum disulfide MoS_2 nanopowder over wide temperature range of 95–350 K

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Abstract

The work is devoted to the study of charge transfer in MoS_2 nanopowder over a wide temperature range. Analysis of the temperature dependence of electrical resistance revealed that three conductivity mechanisms can be found in the studied temperature range. The temperature intervals were established where the mechanisms manifest themselves in their pure form. It was found that at temperatures above 315 K, intrinsic conductivity occurs due to thermal excitation of electrons from the valence band to the conduction band. The temperature range of 230–275 K corresponds to the impurity ionization. The sulfur vacancies act as donor impurity centers. At temperatures below 180 K, charge transfer occurs due to the 3D Mott variable range hopping conduction mechanism. Between the temperature ranges where the mechanisms manifest themselves in their pure form, there are fairly wide transitional temperature ranges where the action of the mechanisms is superimposed. It was found that the band gap for the nanopowder is approximately 1.7 eV, which is higher than in the bulk material (1.2 eV). It is shown that the distance from the donor level induced by sulfur vacancies to the bottom of the conduction band is about 280 meV. The density of localized states near the Fermi levels is about $1*10^{16}$ $cm^{-3}*eV^{-1}$. The characteristic decay length of the wave function (localization length) of a localized charge carrier is about 4 nm. These data are important for biotechnological applications MoS_2 nanoparticles, allowing planning of strategies for using these materials.

Motivation

Molybdenum disulfide MoS_2 attracts attention due to the possibility of its multifunctional application [1-2]. The layered 2D structure of molybdenum disulfide is an inorganic analogue of graphene [3]. MoS_2 hold specific advantages over graphene, including the presence of a bandgap that is critical for electronic and optoelectronic devices. Integrating of semiconductor molybdenum with graphene opens up new possibilities for the development of next-generation, ultrathin, flexible, transparent, light emitting, light-harvesting and light-detecting devices.

Experimental

The studied material of MoS_2 was produced by Sigma Aldrich in form of nanopowder (material No. 804169).
Diameter 90 nm (APS)
Density 5.06 g/mL at 25 °C
The layered 2D structure of molybdenum disulfide are shown in fig. 1. The plan layer of Mo atoms is located between the layers of S atoms. In fact, the Mo atom is located in the center of a triangular prism, at the vertices of which sulfur atoms are present. Electrical measurements were carried out in helium cryostat by two probe method. Temperature stabilization was carried out using Utrecs K43, which allows to control the temperature with an accuracy of 0.01 K.

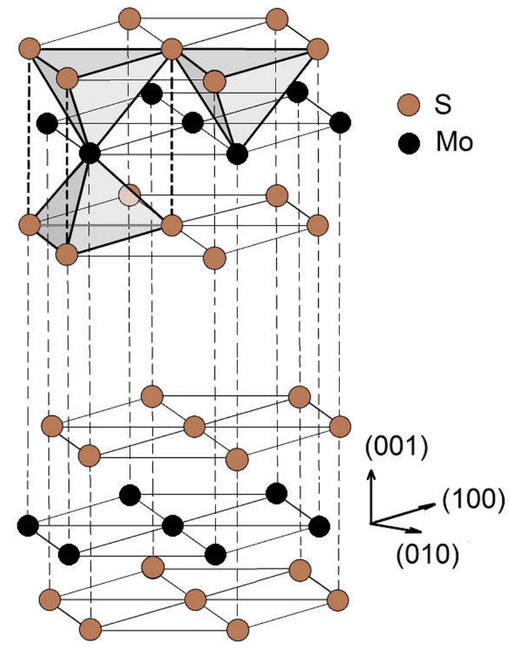

Fig. 1. Crystal structure of molybdenum disulfide MoS2 (see, for example, [1]. The trigonal prismatic coordination of sulfur atoms around the molybdenum atoms in MoS2, within the sandwich layers.

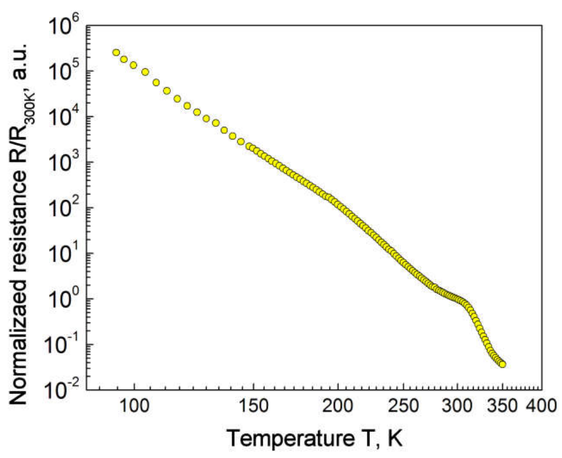

Fig. 2. Temperature dependence of electrical resistance of MoS_2 nanopowder. Data are normalized to resistance at temperature 300 K.

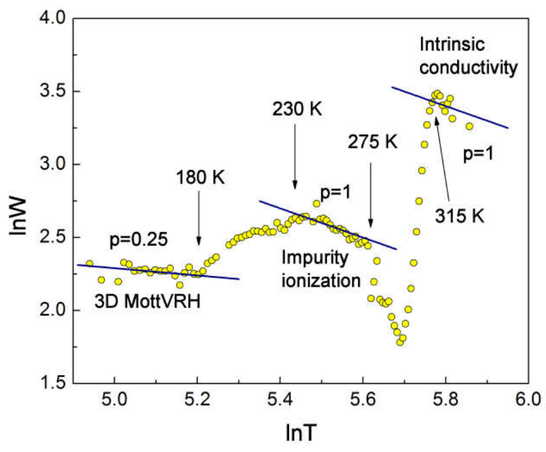

Fig. 3. Temperature dependence of logarithmic derivative *W* on *lnW vs lnT* plot. Straight sections with a negative slope correspond to conduction mechanisms that can be detected in pure form.

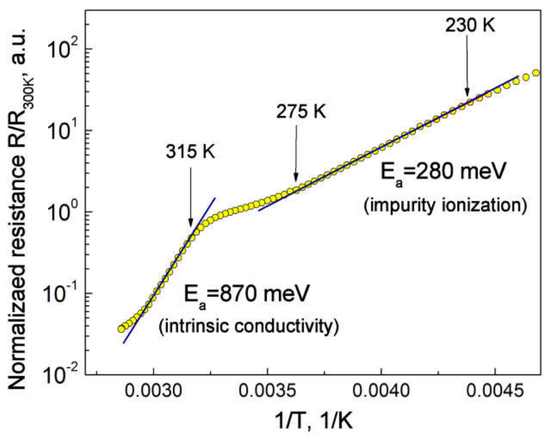

Fig. 4. Dependence of MoS_2 resistance on inverse temperature 1/*T*. The slope of straight sections finds two activation energies, 280 meV and 870 meV, which correspond to temperature ranges of impurity ionization and intrinsic conductivity, respectively.

Results

The resistivity of the investigated sample MoS_2 nanopowder is ~$5*10^3$ Ohm*m at a temperature of 300 K. Reducing the temperature from 350 K to 95 K leads to an increase in resistance by more than seven orders of magnitude (Fig. 2). Resistance curve derivative analysis (RCDA method) was used to find the conduction mechanisms. In accordance with the RCDA method, the temperature dependence of the logarithmic derivative *W* was obtained:

$$W = -\frac{\partial \ln R}{\partial \ln T} \qquad (1)$$

where *R* is a electric resistance, *T* is a temperature.

The *lnW vs lnT* plot contains three straight-line sections with a negative slope (Fig. 3). The slope determines the value of the characteristic index *p*. The index *p* indicates the charge transfer mechanism, and the limits of the linear region find the temperature range where the conductivity mechanism manifests itself in its pure form. Between the linear sections, there are transition ranges where the action of the mechanisms overlaps.

Temperature range above 315 K, characteristic index p=1.

Here, there is intrinsic conductivity due to thermal excitation of electrons into the conduction band and holes into the valence band. The temperature dependence follows the expression:

$$R = R_{0A} \cdot \exp\left(\frac{E_a}{k_B T}\right) \qquad (2)$$

where R_{0A} is the temperature-independent prefactor, k_B is the Boltzmann constant, and E_a is the activation energy of conductivity. For intrinsic conductivity $E_a=E_g/2$, where E_g is the width of band gap. It was found that $E_a \approx 870$ meV (Fig. 4). Therefore, for the studied nanopowder, the band gap width is $E_g \approx 1.7$ eV. The found value is higher than 1.2 eV for bulk MoS_2 [2]. At the same time, 1.7 eV is close to the value of 1.8-1.9 eV reported for monolayers of MoS_2 [3].

Temperature range 230–275 K, characteristic index p=1.

Here, there is impurity conductivity, namely, the region of impurity ionization. The sulfur vacancy probably acts as an electron donor. The temperature dependence also follows expression (2). It was found that the activation energy is $Ea \approx 280$ meV (Fig. 4). The obtained value is in good agreement with the activation energies of 200–300 meV reported for the case of sulfur atom vacancies [4]. The activation energy found is probably approximately equal to the distance from the donor level to the edge of the conduction band. It is because the Fermi level is located within the donor level. Such a Fermi level position is confirmed by the observation of hopping conductivity in the studied samples at temperatures below 180 K.

Temperature range below 180 K, characteristic index p=0.25.

Here, there is variable range hopping conductivity according to the Mott model for the 3D case. The temperature dependence follows the expression:

$$R = R_{0H} \cdot \exp\left(\frac{T_0}{T}\right)^p \qquad (3)$$

R_{0H} is a prefactor that depends weakly on temperature, and T_0 is a characteristic temperature. It was found that $T_0 \approx 3.5*10^8$ K (Fig. 5). In the Mott model, the characteristic temperature is related to the localization length ξ and the density of states at the Fermi levels $N(E_F)$ by the expression:

$$T_0 = \frac{21.2}{k_B N(E_F) \xi^3} \qquad (4)$$

It was found that in the temperature region of hopping conductivity (T<180 K), the resistance of MoS_2 decreases exponentially with increasing applied electric field *E* (Fig. 6). This is explained by the dependence of the prefactor R_{0H} on the electric field *E*:

$$R_{0H} \propto \exp\left(-\gamma \frac{|e|lE}{k_B T}\right) \qquad (5)$$

where $\gamma \approx 1$, *e* is the electron charge, and l is a hopping length. The hopping length is related to the localization length by the expression:

$$l \approx \xi \cdot \left(\frac{T_0}{T}\right)^{1/4} \qquad (6)$$

The slope determined in Fig. 6 and expressions (5) and (6) make it possible to estimate the localization length $\xi \approx 4$ nm. The obtained value of ξ is in good agreement with the published data 2-3 nm of the Bohr radius for the sulfur vacancy in molybdenum disulfide [5]. It was found using expression (4), that the density of states at the Fermi levels is $N(E_F) \approx 1*10^{16}$ $cm^{-3}*eV^{-1}$.

The obtained data allow us to schematically represent the band structure of the studied MoS_2 nanopowder near the Fermi level (Fig. 7).

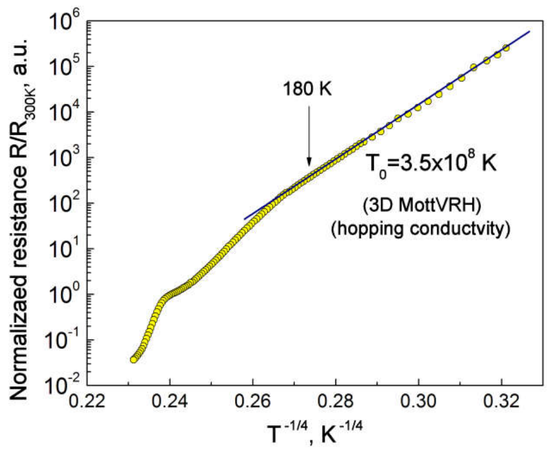

Fig. 5. Dependence of MoS_2 resistance on inverse temperature $T^{-1/4}$. The linear behavior of the experimental data confirms the 3D MottVRH mechanism of hopping conduction below 180 K.

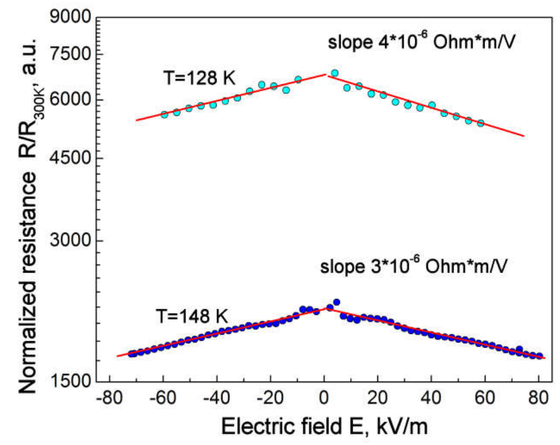

Fig. 6. Dependence of MoS_2 resistance on applied electric field *E*. The linear behavior confirms hopping charge transfer according MottVRH model at low temperatures.

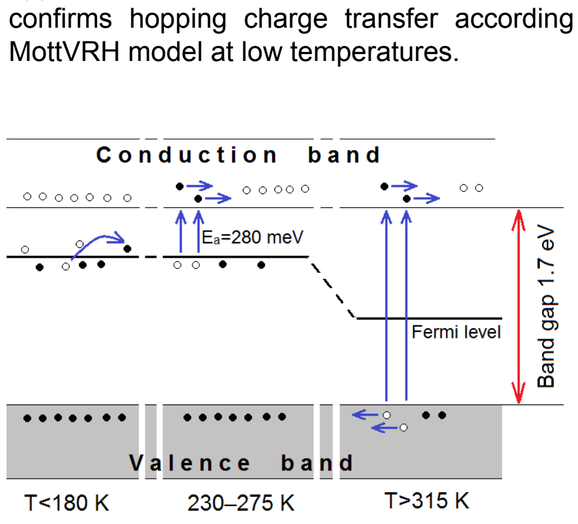

Fig. 7. Schematic band structure of MoS_2 nanopowder and charge transfer mechanisms at different temperatures.

Conclusions

The investigation of charge transfer in the MoS_2 nanopowder made it possible to obtain information about the conductivity mechanisms and the band structure. It was found that the band gap is about 1.7 eV. The donor level induced by sulfur vacancies is 280 meV below the bottom of the conduction band. The density of states at the Fermi level is about $1*10^{16}$ $cm^{-3}*eV^{-1}$. The localization length is 4 nm. These data are important for biotechnological applications MoS_2 nanoparticles, allowing planning of strategies for using these materials.

References

[1] O. El. Beqqali et al, Electrical properties of molybdenum disulfide MoS2. Experimental study and density functional calculation results, *Synthetic Metals* ***90***, 1997, 165.
[2] E. Kim et al, Tuning the optical and electrical properties of MoS2 by selective Ag photo-reduction, *Appl. Phys. Let.* ***113***, 2018, 013105.
[3] D. Liu et al, Sulfur vacancies in monolayer MoS2 and its electrical contacts, *Appl. Phys. Let.* ***103***, 2013, 183113.
[4] S.-T. Lo et al, Transport in disordered monolayer MoS2 Nanoflakes - evidence for inhomogeneous charge transport, *Nanotechnology* ***25***, 2014, 375201.
[5] A. Hötger, *et al.* Spin-defect characteristics of single sulfur vacancies in monolayer MoS_2. *npj 2D Mater Appl* **7**, 2023, 30.