Abstract

Graphene research, distinguished with the Nobel Prize in 2010, opened up a new global field of studies dedicated to atomically thin layered materials (2D materials), which also includes the family of transition metal dichalcogenides. Tantalum disulfide in its 1T polytype (1T-TaS_2) belongs to this family and is a unique material, showing various interesting properties even in its bulk form. Moreover, it can also be used as a part of 2D hybrid structures made of different layered materials, known as NanoLego. 1T-TaS_2 features temperature-dependent phase transitions related to charge density waves. In particular, it undergoes a metal-insulator phase transition, which is accompanied by periodic lattice distortions. A band gap opening together with structural changes can be tracked by means of electrical measurements and Raman spectroscopy.

This work is dedicated to studies on the properties of 1T-TaS_2 in different phases as well as hybrid structures composed of tantalum disulfide and graphene using electrical measurements and Raman spectroscopy. The main purpose of the experiments with graphene/1T-TaS_2 hybrid structures was to study whether graphene's properties can be altered through the proximity effect with 1T-TaS_2.

Chapter 1.1 introduces the field of two-dimensional materials, with the emphasis on transition metal dichalcogenides. Hybrid structures made of different layered materials are also addressed. The next chapter is dedicated to the properties of 1T-TaS_2, including charge density waves, temperature-dependent phase transitions and consequent crystal lattice rearrangement. The dependence of the electrical resistance on temperature illustrating the metal-insulator transition is also shown. Chapter 1.2.3 presents the electronic band structure of 1T-TaS_2 calculated by DFT methods, which is discussed in the context of resonant Raman scattering. Chapter 1.3 elaborates on potential applications of 1T-TaS_2. Chapter 1.4 describes the classical and microscopic theory of Raman scattering and explains the usefulness of Raman spectroscopy for the research on 1T-TaS_2 phase transitions. In Chapter 1.5, the Seebeck effect is described and the dependence of the Seebeck coefficient of 1T-TaS_2 on temperature is presented, which is relevant in terms of simultaneous electrical and Raman measurements.

Chapter 2 is dedicated to experimental details. Firstly (Chapter 2.1), sample preparation is described. Then (Chapter 2.2), experimental Raman scattering setups are presented, in particular the setups used for polarization-resolved measurements. In Chapter 2.3, the experimental setup allowing for electrooptical measurements is described. Chapter 2.4 introduces principal component analysis (PCA) and explains how it is employed in the analysis of the results presented in this work.

Experimental results are presented in Chapter 3. Firstly (Chapter 3.1.1), the impact of phase transitions on 1T-TaS_2 Raman scattering spectra is discussed, including the temperature dependence of low- and high-temperature components. The next chapter (3.1.2) focuses on the hysteresis of the metal-insulator phase transition, which is studied by simultaneous optical and electrical measurements. These studies demonstrate noticeable differences between the hysteresis determined based on electrical resistance and Raman scattering measurements. Chapter 3.2 addresses the impact of laser irradiation, used for Raman scattering experiments, on the electrical response of 1T-TaS_2. An additional voltage due to laser light was observed, which was interpreted as Seebeck effect. This phenomenon was used in order to create spatially resolved maps of thermoelectric voltage. The maps show that it is possible to achieve a metastable state of 1T-TaS_2, which is a mixture of metallic and insulating states existing at the same time. The coexistence of different phases was confirmed by appropriate Raman scattering measurements. This result is important regarding both potential applications (e.g. memristors) and the understanding of phase transitions in layered materials with charge density waves.

In Chapter 3.3 the 1T-TaS_2 Raman scattering spectra dependence on the excitation energy is presented. Considerable differences in the relative intensity of Raman modes due to different excitation energy were observed. The obtained results are discussed in terms of resonant effects, resulting from interaction between laser irradiation and electronic states of the investigated sample.

In the next chapter (3.4) polarization-resolved Raman scattering spectra of 1T-TaS_2 are presented. According to our best knowledge, full angular dependencies were measured for the first time. Theoretically predicted angular plots for scattered light polarization and laser light polarization with respect to the sample orientation are shown. However, it turns out that the theory widely used for polarization resolved Raman spectra analysis does not explain the obtained results. The observed effect resembles phase transitions in a ferromagnetic system, where the linear polarization angle of a Raman mode can be altered by switching the sample magnetization. The measured linear polarization dependencies can be described by an antisymmetric tensor used for the analysis of Raman optical activity. Consequently, we postulated that 1T-TaS_2 shows Raman optical activity, which was confirmed by measurements in circularly polarized light. A connection between the linear polarization axis and the behaviour of Raman modes excited with circularly polarized light was found. The three main observed linear polarization axis angles were related to the folding of the first Brillouin zone accompanying the structural rearrangement during metal-insulator phase transition. In the presented research the Raman optical activity of 1T-TaS_2 was observed for the first time.

In Chapter 3.5 the results of Raman scattering measurements of epitaxial graphene/1T-TaS_2 hybrid structures are presented. Spatially resolved Raman scattering maps proved an interaction between graphene and tantalum disulfide, in particular a charge carrier transfer was observed. This result is a precursor to further research, which would explore the inducement of spin-orbit coupling in graphene through the proximity effect, which is very attractive regarding applications in spintronics. The obtained results suggest that it is crucial to prepare graphene/1T-TaS_2 hybrid structures in an inert atmosphere in order to observe the interaction between these two materials, because the interface between graphene and tantalum disulfide needs to be protected from oxidation.

Chapter 4 constitutes the summary of this thesis. It also discusses research directions, which could provide further insight into the investigated subject matter.