Report on the outcomes of a Short-Term Scientific Mission[1]

Action number: CA21126

Grantee name: Olesia Romantsova

Details of the STSM

Title: Thermodynamic properties of materials containing hydrated fullerene inclusions at extra low temperatures

Start and end date: 10/01/2025 to 31/01/2025

Description of the work carried out during the STSM

(max. 500 words)

The study investigated the heat capacity of thermally reduced graphene oxide (TRGO) combined with fullerene C60 (HyFn) within the temperature range of 2 K to 300 K using the thermal relaxation method via a Physical Property Measurement System (PPMS) equipped with a Heat Capacity Module. In addition to these materials a reference tests with commercial samples from Sigma Aldrich were performed both for pure fullerene C60 and graphene oxide. The research focused on the heat transport properties of various materials that exhibited disordered characteristics at low temperatures, aiming to identify and understand specific anomalies in their thermal behavior.

Throughout the study, several complementary experiments were conducted alongside heat capacity measurements to gain a comprehensive understanding of the thermal behavior of these materials:

- X-ray diffraction (XRD) measurements to determine the crystallographic structure and phase composition,
- Raman spectroscopy measurements to analyze vibrational modes, bonding, and molecular interactions,
- Transmission electron microscopy (TEM) pictures to get the insight into the sample microstructure
- comparative analysis of TRGO-HyFn composites and pure fullerene C60 to assess the influence of molecular interactions on heat capacity.

A key objective was to explore how structural disorder influences the emergence of characteristic anomalies in heat capacity, such as the boson peak, which appeared in the temperature dependence. This anomaly, commonly associated with the vibrational density of states in disordered systems, is crucial for understanding the low-temperature thermal properties of nanostructured materials. By

[1] This report is submitted by the grantee to the Action MC for approval and for claiming payment of the awarded grant. The Grant Awarding Coordinator coordinates the evaluation of this report on behalf of the Action MC and instructs the GH for payment of the Grant.

investigating these characteristics, the study provided deeper insights into how disorder affects heat transport mechanisms in complex carbon-based systems.

The investigation primarily involved X-ray diffraction (XRD) and Raman spectroscopy measurements, which provided a detailed physical insight into the structural and vibrational characteristics of these compounds. XRD delivered precise information on crystallographic structure and phase composition, confirming the presence of specific phases and their stability at low temperatures. Raman spectroscopy identified vibrational modes, bonding characteristics, and molecular interactions within the material, allowing for an in-depth analysis of lattice dynamics and disorder-induced effects. Combined, these techniques helped clarify how structural order, lattice dynamics, and molecular interactions influenced heat capacity and thermal transport mechanisms, leading to a more comprehensive understanding of thermal behaviour in these nanostructured composites. Additional investigations including the transmission electron microscopy of both samples obtained at my Home Institute and the commercial ones have exposed the differences in structure stemming from the synthesis procedure.

The experimental results were analyzed using both phenomenological and theoretical models, such as the soft-potential model and the Debye model. These theoretical approaches allowed for the interpretation of observed anomalies and the establishment of correlations between structural disorder and heat capacity behaviour. The findings laid the foundation for further advanced research, contributing to a deeper understanding of disordered systems and their thermal properties at low temperatures. This knowledge is particularly relevant for applications in nanotechnology and cosmic science, where thermal management and heat dissipation play a critical role in device performance and material stability.

Description of the STSM main achievements and planned follow-up activities

Description and assessment of whether the STSM achieved its planned goals and expected outcomes, including specific contribution to Action objective and deliverables, or publications resulting from the STSM. Agreed plans for future follow-up collaborations shall also be described in this section.

(max. 500 words)

The objective of this proposal was to verify and further explore the distinctive features identified in low-temperature heat capacity studies in low-dimensional carbon-based systems. These materials, including graphene oxide and fullerene, were of particular interest due to their unique structural and thermal properties. The goal was to gain a better understanding of the type of disorder present in these systems and how it influenced their thermal behavior.

During the research stay, TRGO-HyFn composites and pure fullerene sample were systematically investigated. The heat capacity measurements revealed a pronounced boson peak in the data for the fullerene sample and the composite, but none for the graphene oxide, indicating significant thermal anomalies associated with their structural and vibrational properties.

These effects were especially significant at extremely low temperatures, below 10K, conditions that closely resemble those found in space. Another reason for conducting experiments on composites of graphene oxide with fullerene inclusions by analyzing heat capacity temperature relations was the necessity of performing thermal studies in high vacuum, which effectively mimicked the extraterrestrial environment. Based on the data obtained, it is planned to write an article with the detailed analysis of the results. I was also invited to give a seminar at the Host Institution in future. The results will be also presented in the upcoming conference held in June at my Home Institute - CMLTP

The study provided a detailed and quantitative description of the physics and chemistry of cosmic carbon nanomaterials, aligning with the main objective of the Action as initially outlined in the research coordination framework. Given the circumstances in Kharkiv, where fundamental activities at the Home Institution were significantly hindered, maintaining collaboration, accessing research facilities, and ensuring continued progress through joint research and proposals became increasingly important. Last but not least, another key aspect of the realized STSM was also fostering knowledge exchange

between researchers from the Home and Host Institutions.