Experimental report

16/02/2026

Proposal: **6-05-1069**

Council: 4/2023

Title: Anomalous low-temperature conductivity of As-S glasses

Research area: Physics

This proposal is a new proposal

Main proposer: **JOZEF BEDNARCIK**

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Samples: As29S71
As50S50

Instrument	Requested days	Allocated days	From	To
D4	3	3	12/11/2023	15/11/2023

Abstract:

The aim of this project is to verify our assumption that the universal anomalous low-temperature properties of the glasses can originate from various types of nanoclusters presented in the As-S glassy matrix. Depending on the sample's composition, it is possible to change the representation of individual nanoclusters characterized by different sizes, topology, and a number of connection points to the glassy matrix. Two samples were selected as the limiting case for the indication of a dominant nanocluster, sulfur-rich sample As29S71 and arsenic-rich sample As50S50. It is expected that ring-like S8 nanoclusters may dominate the As29S71 and nanoclusters with As¿As homo-nuclear bound in As50S50. The main motivation is to directly prove the presence of individual nanoclusters types in the As-S glassy structure and identify each nanocluster representation. Neutron pair distribution function (PDF) technique will be used to quantitatively describe short and medium range order of selected As-S glassy materials. Special emphasis will be placed on a study of their local atomic structure at low temperatures (2-20 K) where they show anomalous behavior of thermal conductivity.

Anomalous low-temperature conductivity of As-S glasses

Proposal ID: 89450

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Instrument: D4 at ILL,

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Dates: 12.-15.11.2023

This project investigates the microscopic origin of the anomalous low-temperature physical properties of arsenic–sulfur (As–S) glasses, focusing on their unusual transport behavior below 30 K. We hypothesize that these anomalies arise from the presence of distinct types of nanoclusters embedded within the disordered As–S matrix. By tuning the glass composition, the distribution, topology, and connectivity of these nanoclusters can be systematically varied, enabling identification of specific structural motifs responsible for low-energy excitations.

Two glass compositions were selected as limiting structural cases: the sulfur-rich $As_{29}S_{71}$ and the arsenic-rich $As_{50}S_{50}$ glass. These materials are expected to favor different dominant nanocluster architectures. Contrasting their temperature-dependent structural evolution provides a route to linking composition-driven nanoscale heterogeneity with anomalous low-temperature conductivity.

Neutron total scattering measurements were performed in situ at low temperatures (5–30 K) on the **D4 diffractometer at the Institut Laue-Langevin (ILL)**. The wide momentum-transfer coverage up to **q_{max} = 22.5 Å^{-1}** enabled high-resolution PDF analysis. The obtained neutron data revealed the presence of **distinct crystalline peaks in the $As_{29}S_{71}$ sample**, suggesting partial nanocrystallization or a tendency toward long-range ordering in this sulfur-rich composition, providing an additional structural contrast between the two glasses. On the other hand, fully amorphous structure was confirmed for the $As_{50}S_{50}$ glass.

To strengthen the structural interpretation and provide independent constraints for the ongoing **Reverse Monte Carlo (RMC) simulations**, **both samples were also measured using in-situ low-temperature EXAFS**. These complementary local-structure datasets will ensure physically meaningful RMC models and help identify composition-dependent nanocluster characteristics.

Together, the neutron and EXAFS results are expected to significantly improve our understanding of how nanoscale structural motifs govern the universal anomalous low-temperature properties of chalcogenide glasses. **At the moment, we are building a suitable structural model for the RMC modelling of the $As_{50}S_{50}$ sample.**