Determination of Short- and Intermediate Range Atomic Structures in Amorphous GST-Materials via Anomalous X-ray Scattering

J. R. Stellhorn[1] , W.-C. Pilgrim[1], A. Höhle[1] , S. Hosokawa[1,2]

[1] FB Chemie, Physikalische Chemie, Philipps-Universität Marburg, 35032 Marburg, Germany
[2] Department of Physics, Kumamoto University, Kumamoto 860-8555, Japan

ABSTRACT

Key words: GST, Anomalous scattering, AXS, amorphous.

This project aims at determining the partial structural properties of the amorphous phases of alloys of the family $(GeTe)_{1-x}(Sb_2Te_3)_x$ by utilizing a combination of anomalous x-ray scattering (AXS) experiments and reverse Monte-Carlo (RMC) modeling [1]. The AXS-method exploits the strong change in the real part of the form factor closely below an absorption edge and provides the differential structure factors $\Delta_k S(q)$, which indicate the environment around a specific atomic species in high accuracy. Through a subsequent RMC simulation, the need for a complete set of equations to solve the correspondent scattering matrix for all partial correlations can be overcome, as other physical and chemical constraints (e.g. minimum atomic distances or bond angles due to known electronic properties) can be included into the RMC scheme [2, 3, 4]. Thus, a detailed picture of the short and intermediate range order in form of (partial) pair distribution functions is obtained, which can be used to understand the structural transformations during the fast crystalline/amorphous transition in the GST-family (see, e.g. [1]).

Employing the obtained RMC simulation results on GST-2,2,5, it was recently possibly to refine the view of the "umbrella flip" phase change mechanism suggested by Kolobov [5]. Additionally, it was possible to proof the existence of Ge-Ge-bond chains and of Ge-Te-Ge-Te fourfold puckered ring structures (cf. fig. 1, taken from [1]).

Comparative AXS-measurements on the GST family $(GeTe)_{1-x}(Sb_2Te_3)_x$ also indicate that GeTe (x=0), GST-8,2,11 (x=1/9) and GST-2,2,5 (x=1/3) exhibit common features in their structure; though we have conducted only preliminary measurements on GST-8,2,11 until now. Most notably we find evidence for the "pre-peak" at about 1 $Å^{-1}$ in the differential structure factors at the Ge-adsorption edge in all cases, indicating an intermediate range order based on the Ge atoms.

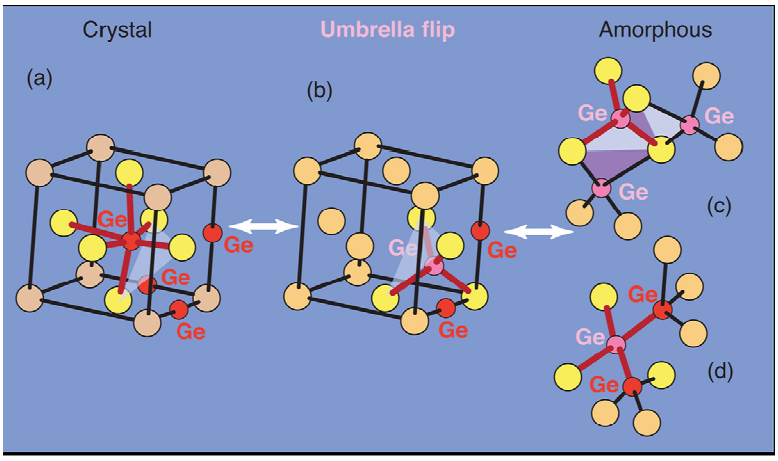

Fig. 1: The modified “umbrella flip” picture depicting the origin of Ge-bond chains and Ge-Te-Ge-Te ring structures.

REFERENCES

1. S. Hosokawa et al., J. Appl. Phys. **111** (2012) 083517

2. W.-C. Pilgrim, J. R. Stellhorn, S. Hosokawa, Bunsenmagazin **15** (2013) 131-145

3. S. Hosokawa et al., Int. J. Mat. Res. **103** (2012) 1108

4. O. Gereben, P. Jóvári, L. Temleitner, L. Pusztai, J. Optoelectron. Adv. Mater. **9** (2007) 3021-3027

5. A. V. Kolobov et al., Nat. Mater. **3** (2004) 703-708

6. J. Akola, R.O. Jones, Phy. Stat. Solidi **249** (2012) 1851-1860

Biographies

Jens R. Stellhorn is a PhD student at the Philipps University of Marburg, Germany, in the group of Prof. Pilgrim. He received his Master’s degree in physical chemistry at the Philipps University in 2012 and since then his field of research is concerned with the determination of the structures in amorphous materials using Anomalous X-Ray Scattering.