ESRF	**Experiment title:** Intermediate range order in the new phase-change material GeCuTe2	**Experiment number**: **HC-2534**
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Report:

The GeTe-CuTe system (GCT) has been proposed as a new phase change material (PCM) class, and it is expected to be used for a next generation of data storage (non-volatile) memories instead of the usual Ge-Sb-Te (GST) alloys. In particular, the composition $Ge_1Cu_1Te_2$ is of special interest for electronic memories, as it possesses a considerable electrical contrast between the amorphous and the crystalline phase while offering a negligible change in the macroscopic density [1], thereby greatly enhancing the life-time and cyclability of the data carrier. To elucidate the structure-property relations in this amorphous compound, we conducted anomalous X-ray scattering (AXS) experiments close to the *K*-edges of all the constituent elements. In combination with the use of reverse Monte Carlo modelling, we are able to characterize the short- and intermediate-range atomic structures (SRO and IRO, respectively).

GCT crystalline films were found to be easily amorphised by laser irradiation with a lower power and short pulse width [2], which are essential properties to achieve rapid data recording and low power consumption in a PCM. In contrast to widely studied PCMs like GST, amorphous Ge-Cu-Te compounds exhibit a complex compositional dependence of the phase-change properties like the density change or the optical contrast ΔR_{opt}. In the case of $Ge_1Cu_1Te_2$, these two properties are close to zero, while taking negative values for higher contents of Cu. On the other hand, a considerable electrical contrast between the amorphous and crystalline phase remains even in $Ge_1Cu_1Te_2$, rendering it suitable for PCM applications.

Despite its significance among the GCT PCMs, the composition $Ge_1Cu_1Te_2$ proposed for the experiment herein has not yet been subject to experimental or theoretical investigations. However, it may represent the cornerstone to develop a new concept to understand the optical contrast in PCMs. This property has been described for the Ge-Sb-Te system and was understood to arise from a large difference in the optical matrix elements [3], i.e. these are enhanced in the crystal by aligned rows of resonantly bonded *p*-orbitals, while the amorphous phase has no enhancement due to an absence of this order. This model alone however cannot explain the complex dependence of ΔR_{opt} in GCT, so that a new concept is necessary to understand the structure-property relations.

The experiment results indicate that no sudden jump in the structure of the amorphous phase occurs along the pseudo-binary line GeTe-CuTe, as it is observed for the crystalline phases. But there are distinct changes in the short- and intermediate-range order, which can be visualized by comparison with structural results of $GeCu_2Te_3$ and GeTe, which our group has already investigated by AXS. The resulting total structure factors are shown in fig. 1. Apparently, all total $S(Q)$ functions show large similarities, only the second main peak around 3.2 $Å^{-1}$ is steadily increasing in intensity an shifting towards lower Q values as a function of the CuTe content. Furthermore, the low-Q signal exhibits an increasing trend. Both characteristics are crucial to understand the structure-property relationships in the GCT system.

The in-depth analysis of the intermediate-range order is still ongoing, but even this preliminary analysis shows the importance of determining the content-dependence of structural features to clarify the structure-property relations. Thus, further experiments are planned to study the GCT system, with special regard to $Ge_4Cu_1Te_5$ (containing 20 atom% CuTe), as it exhibits the highest temperature of crystallization in the entire GeTe-CuTe system, but shows a phase-change density change and optical contrast comparable to GeTe. [1,2]

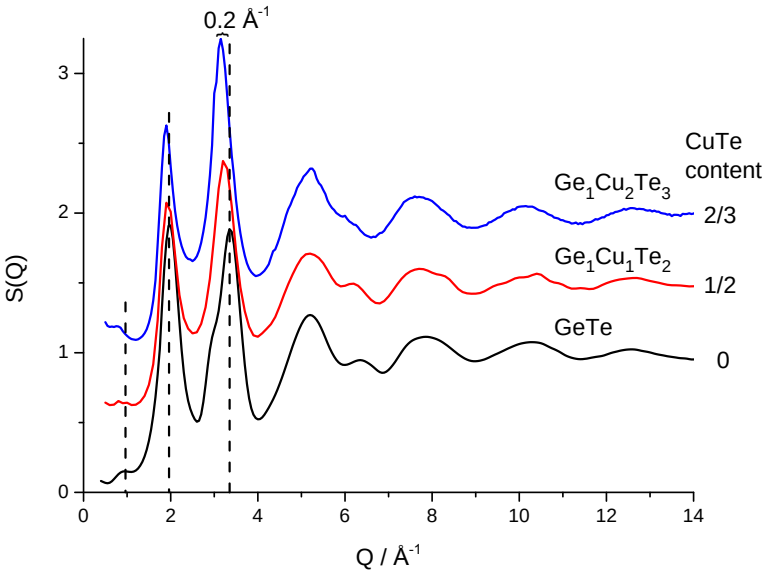

Fig. 1: Total structure factors of $Ge_1Cu_1Te_2$, in comparison with previous results on GeTe and $GeCu_2Te_3$.

References

[1] Y. Saito et al., J. Phys. Chem. C. **118**, 26973 (2014).

[2] Y. Saito et al., Appl. Phys. Lett. **102**, 051910 (2013).

[3] B. Huang and J. Robertson, Phys. Rev. B **81**, 081204(R) (2010).