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Report:

$GeCu_2Te_3$ (GCT) is a new phase change material (PCM), which is expected to be used for a next generation of data storage (non-volatile) memories, instead of the currently employed Ge-Sb-Te (GST) alloys. Both systems utilise the amorphous-crystalline reversible phase change to encode binary data. However, GCT shows more promising feautures like a lower power consumption and a smaller density change during the phase-change process. Futhermore, GCT exhibits a *negative* optical contrast, i.e., the reflectivity in the crystalline phase is lower than that in the amorphous phase [1], in opposition to commonly used PCMs such as GST with a positive optical contrast.

So far, the state of research on the atomic-scale structure is inconsistent: different average coordination numbers have been reported by x-ray diffraction in combination with XAFS measurements [2], by XAFS investigations [3] and by *ab-initio* MD [4]. Experimental data claim that all atoms are roughly fourfold coordinated, which would constitute a large similarity to the tetrahedral crystal structure. MD simulations range the coordination number of Ge and Cu much larger, with values exceeding 6 for Cu and ~4.5 for Ge.

To investigate the structure-property relations in amorphous GCT, 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 (RMC) modelling, the experimental data can determine the short- and intermediate-range structural characteristics. The resulting $\Delta_k S(Q)$ functions and RMC fits are illustrated in fig. 1.

An excellent agreement is obtained between experimental data and the RMC model. Coordination numbers are much higher than reported in [2] by EXAFS measurements. Instead, they are much closer to theoretically

predicted values [4], and are as large as N(Ge) = 4.8 and N(Cu) = 5.2. Even Te adopts a high coordination number of 3.9. Furthermore, a very high number of homopolar bonds is found.

The larger coordination numbers are in agreement with the experimentally found higher density of the amorphous phase compared to the crystal, which is another unusal characteristic of the GCT phase-change process. The large coordination numbers also neccesitate bond angles smaller than the ~109° angles, which are found for the tetrahedral arrangements in the crystal. The increased number of smaller bond angles consequentially have a pronounced impact on the intermediate-range order. Recent AXS experiments by our group have shown that the optical contrast in the system Ge-Sb-Te can be satisfactorily explained by taking into account the character of the intermediate-range order [5]: An octahedral network, i.e. bond angles close to 90°, on the intermediate length level can be interpreted as being responsible for an increasing optical permittivity, in a similar way as proposed for the crystalline phase. Thus, the results for GCT are in line with the trend found for GeSbTe phase-change materials, where a more tetrahedral network structure appears to diminish the dielectric constant and concomitantly the reflectivity of the *crystal*, thus explaining the negative optical contrast in GCT.

Correlation	Amorph.	Cryst.
GeGe	1.4	
GeCu	1.5	
GeTe	1.9	4
CuCu	2.3	
CuGe	0.7	
CuTe	2.1	4
TeGe	0.6	1.3
TeCu	1.4	2.7
TeTe	1.9	
N_{Ge}	4.8	4
N_{Cu}	5.2	4
N_{Te}	3.9	4
$N_{average}$	4.5	4

Tab. 1: Partial and total coordination numbers extracted from the partial pair correlation functions obtained from the RMC models, in comparison with values for the crystalline phase [6].

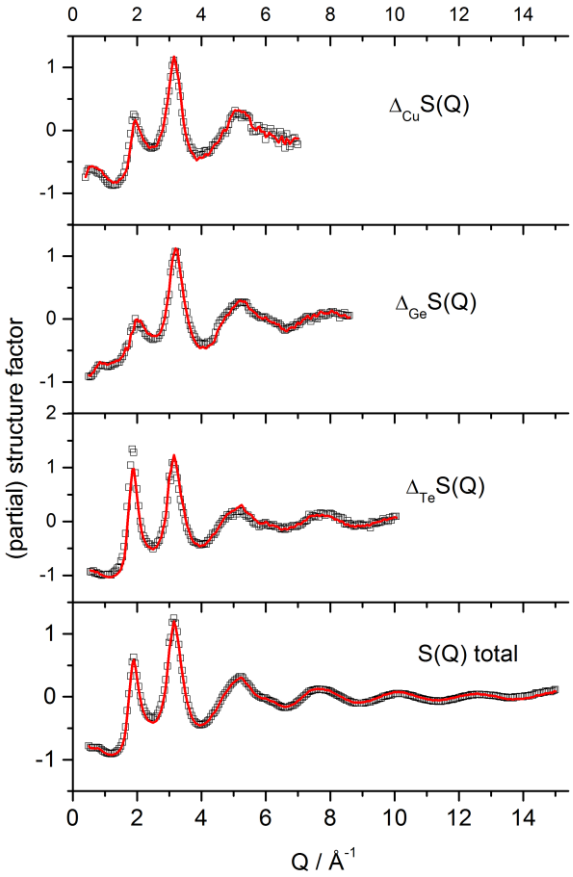

Fig. 1: Experimentally determined $\Delta_k S(Q)$ functions (squares) and RMC fits (red lines).

References

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