

Presentation: Oral

Title: Structural changes of c/a- $\text{Ge}_2\text{Sb}_2\text{Te}_5$ due to RMC analysis with EXAFS and XRD data

Presented by:

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Abstract: GeSbTe compounds are one of the most popular materials for phase change optical recording because of the fast transition rate from a crystalline to an amorphous solid and the cyclability. However the structures of the crystalline and amorphous state are not yet completely understood for the explanation of the fast transition rate. A reverse Monte Carlo analysis can answer this kind of problem. We have obtained numerical data by XRD experiment for the crystalline film and powder diffraction and EXAFS experiments for amorphous film. In order to make an initial configuration for a- $\text{Ge}_2\text{Sb}_2\text{Te}_5$ we start RMC for c- $\text{Ge}_2\text{Sb}_2\text{Te}_5$ with a convoluted XRD data to a small size. Then RMC analysis for a- $\text{Ge}_2\text{Sb}_2\text{Te}_5$ was carried out using three EXAFS spectra from each edge of species. We found that a structure in shorter distances is finely obtained due to EXAFS spectra, which is in reasonable agreement with previous works. However it could not be produce the configuration as a few Monte Carlo steps as it can explain the fast transition rate. We think the problem is in the structure of the crystalline state.