Structural change upon annealing of amorphous GeSbTe on Si(111)

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ABSTRACT

The structural change upon annealing of an amorphous GST film deposited by molecular beam epitaxy (MBE) on a Si(111) substrate is studied by means of X-ray diffraction (XRD), X-ray reflectivity (XRR) and atomic force microscopy (AFM). XRD profiles reveal that both metastable cubic and stable hexagonal phases are obtained with a single out-of plane orientation of the grains.

Key words: GST, crystallization, Si (111) substrate, crystal structure, X-ray diffraction

Effects of thermal crystallization on the structure of GeSbTe (GST) alloys have been widely studied.[1–4] In general the films used in those investigations are produced by sputtering technique and grown on Si substrates with native SiO_2. The resulting phase is thus polycrystalline. Here we present a study of the crystallization of a 20 nm thick GST amorphous film grown on a crystalline 7x7-Si(111) substrate by MBE. The film, deposited at RT, has been annealed for increasing temperatures in a rapid thermal annealing furnace in nitrogen atmosphere (1000 sccm) and after each annealing, the structure has been investigated by means of XRR, XRD and AFM.

Figure 1 shows XRD scans performed on the sample after annealing at different temperatures (T). Both metastable cubic phase (*Fm-3m*) and hexagonal phase (*R-3m*) are obtained. The crystallization process starts at T = 110 °C and is completed at T = 130 °C. The lattice parameter determined for the cubic phase at T = 125 °C is $a = 5.99$ Å. Since XRD profiles show only Bragg peaks due to the (111) direction it can be concluded that an out-of plane texture is present. AFM images show no appreciable changes in the roughness and morphology of the surface. This suggests that the crystallization process starts and develops in the amorphous film, probably at the interface between the crystalline substrate and the amorphous GST, in contrast to the crystallization of polycrystalline films.[2] Starting from T = 230 °C a hexagonal phase with *c*-plane normal to the substrate direction appears.[5] The out- of plane lattice parameter is $c = 41$ Å. Above T = 300 °C material desorption becomes relevant changing considerably the porosity of the film. XRR profiles show a decrease of thickness and increase of density upon annealing, consistent with previous studies.[1–4]

In conclusion the present investigation demonstrates that both metastable and stable crystalline phases can be obtained by annealing an amorphous GST film deposited by MBE on a Si(111) substrate. XRD profiles show that the substrate and the film share an out of plane epitaxial relationship: for the metastable phase $(111)_{Si}$ // $(111)_{GST}$ and for the hexagonal phase $(111)_{Si}$ // $(0001)_{GST}$, respectively. AFM images suggest that the nucleation starts and develops inside the GST amorphous matrix, or most probably at the interface between the film and the Si(111) substrate, which acts as an epitaxial template. Analysis of the XRR curves suggests a decrease in thickness and increase of the GST density with increasing annealing temperatures, in agreement with previous studies.

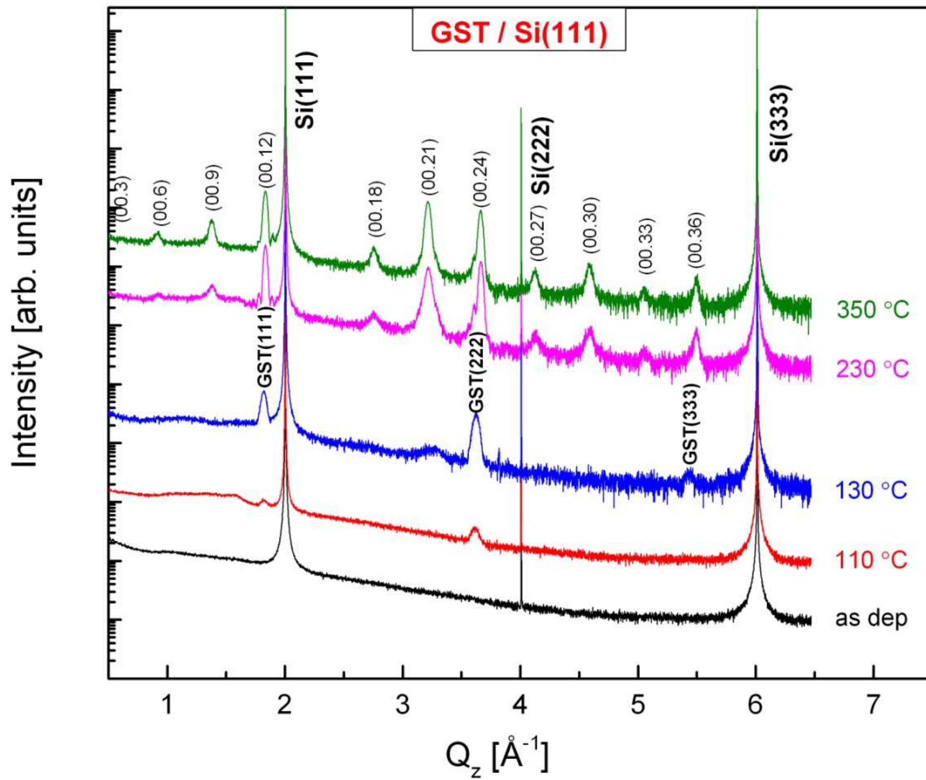

Figure 1: XRD profiles for GST / Si(111) for as-deposited and increasing temperature of annealing T [˚C].

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