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Atomic crystal structure of ordered In$_3$Sb$_1$Te$_2$ ternary alloy studied by high-resolution transmission electron microscopy

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The atomic structure of In$_3$Sb$_1$Te$_2$ was investigated by high-resolution transmission electron microscopy (HRTEM) and the National Center for Electron Microscopy Simulation System. In$_3$Sb$_1$Te$_2$ has a disordered NaCl structure; In atoms are positioned in a face-centered cubic lattice, and Sb and Te atoms are located at randomly occupied octahedral sites. However, the observed HRTEM images of the ordered In$_3$Sb$_1$Te$_2$ phase show that Sb and Te atoms are located in specific positions, that is, at the center and edge of the unit cell, respectively. The atomic model of the ordered In$_3$Sb$_1$Te$_2$ is confirmed by simulated images, which match the experimental HRTEM images. © 2012 American Institute of Physics. [http://dx.doi.org/10.1063/1.3702575]

Phase change random access memory (PRAM) based on chalcogenide alloys has attracted much attention for next generation non-volatile memory due to its fast operation, high scalability, and low fabrication costs. A remarkable generation non-volatile memory due to its fast operation, chalcogenide alloys has attracted much attention for next age density. To solve these issues, many researchers have demand for an improvement in power consumption and stor-...
parameter $a_0 = 6.12$ Å. The In$_3$Sb$_1$Te$_2$ ternary alloy consists of In atoms in face-centered cubic (fcc) sites and Sb and Te atoms occupying the octahedral sites, respectively. The HRTEM image and corresponding fast Fourier transform (FFT) pattern of the In$_3$Sb$_1$Te$_2$ phase are shown in Fig. 1(c). Along the [011] zone axis, the lattice contrast of the HRTEM image should be uniform for all atomic sites. Because the Sb and Te atoms occupy the same atomic positions, the HRTEM and the FFT pattern (inset) indicate that a superlattice phase does not exist. In addition, it was reported that the superlattice structure was not observed in In$_3$Sb$_1$Te$_2$ nanowires synthesized by a metal-organic chemical vapor deposition (MOCVD). The nanowires were grown at a low temperature of 250°C and high working pressures of $13 \times 10^2$ Pa. From the TEM analysis, it was confirmed that the crystal structure of the nanowires was consistent with the structure of the IST thin film annealed at 450°C for 10 min. Therefore, we conclude that In$_3$Sb$_1$Te$_2$ assumes the disordered NaCl structure like metastable GST.

Figure 2(a) shows a BFTEM image of an IST thin film annealed at 450°C for 60 min. The In$_3$Sb$_1$Te$_2$ grains in the film are 50–100 nm in size. Figures 2(b) and 2(d) show BFTEM images of the edge region of the thin film. The corresponding SAED patterns are observed along the directions of the [011] and [012] zone axes as shown in Figs. 2(c) and 2(e), respectively. One of the most interesting findings in this experiment is the extra spots, which are marked with yellow color in the figures (100, 011, 221, 121, 021, and so on). The original diffraction spots in the In$_3$Sb$_1$Te$_2$ ternary alloy are 111, 200, 022, and so on. Compared with the FFT pattern along the [011] zone axis, the 100 and 011 spots should not be found in the NaCl structure of the In$_3$Sb$_1$Te$_2$ phase, as shown in the inset of Fig. 1(c). Generally, reflections possibly present, but their intensity is different, if $h$, $k$, and $l$ which are the Miller indices of a plane are unmixed. Thus, reflections occur for such planes as (111), (200), and (220) but not for the planes (100), (011), (021), and so on in the In$_3$Sb$_1$Te$_2$ phase. From this result, it is clear that the atomic structure of In$_3$Sb$_1$Te$_2$ has a periodical arrangement of Sb and Te atoms, because for an ordered material there will be superlattice reflections at the positions which are forbidden for the disordered structure.

To reveal more structural details of the In$_3$Sb$_1$Te$_2$ crystal, we present HRTEM images along the [011] and [012] directions in Figs. 3(a) and 3(b), respectively. The HRTEM images show the different lattice contrast with an array of bright and dark lines that come from the superlattice reflections. Extra diffraction spots are also observed in the FFT images of the insets. The crystal structure appears to possess a certain periodic relationship between Sb and Te atoms. We suppose that In atoms are not changed in the fcc sites, whereas Sb and Te atoms are located at specific positions among the octahedral sites. The interplanar spacing of (200) is 3.06 Å, which is the same as for the disordered crystalline phase of In$_3$Sb$_1$Te$_2$, but the distance of the (100) plane increases to 6.12 Å, which is double the spacing of the (200) plane, without a change in lattice parameter. The atomic arrangements along the [011] and [012] zone axes are illustrated in Figs. 3(c) and 3(d), respectively. In the [011] projection of the disordered In$_3$Sb$_1$Te$_2$ structure, Sb and Te...
atoms overlap each other randomly. However, the (100) and (200) planes are occupied with the different stacking sequence in the ordered In$_3$Sb$_1$Te$_2$ phase, as shown in Fig. 3(c). The contrast difference in the HRTEM image occurs due to the stacking sequence of -Te-Te- or -Te-Sb-. We also present the atomic arrangement of the [012] zone axis in Fig. 3(d). The atomic sequences in the [012] direction are -In-Te- and -In-Sb-.

The atomic structure model of ordered In$_3$Sb$_1$Te$_2$ is described in Fig. 4(a). The construction is based on the atomic arrangements along the [011] and [012] directions, as shown in Figs. 3(c) and 3(d), respectively. While In atoms occupy a fcc lattice, Sb and Te atoms are located at the center and edge of the unit cell, respectively. In order to verify the atomic structure of the ordered In$_3$Sb$_1$Te$_2$, simulations of the HRTEM image and SAED patterns were performed using the NCEMSS software. We carried out the HRTEM simulations as a function of defocus and thickness based on the model, as shown in Fig. 4(a). Figures 4(b) and 4(c) show the simulated HRTEM images and corresponding electron diffraction patterns, respectively. The simulated HRTEM image was obtained using a defocus of 44 nm, a thickness of 10 nm, and the [011] zone axis, as shown in Fig. 4(b), and the results are consistent with the experimental HRTEM image shown in Fig. 3(a). Similarly, Fig. 4(c) shows the simulated HRTEM image along the [012] beam direction using a defocus of 55 nm and a thickness of 25 nm. It also matches the observed HRTEM images well, as shown in Fig. 3(b).

In summary, we have investigated to understand the atomic structure of the In$_3$Sb$_1$Te$_2$ ternary alloy using HRTEM and NCEMSS. According to the different annealing times, disordered and ordered In$_3$Sb$_1$Te$_2$ phases are observed. The disordered In$_3$Sb$_1$Te$_2$ has the NaCl structure which consists of Sb and Te atoms randomly occupying the octahedral sites, whereas the ordered In$_3$Sb$_1$Te$_2$ has Sb and Te atoms located at the center and edge of the unit cell, respectively. The 3-dimensional atomic structure model of the ordered In$_3$Sb$_1$Te$_2$ phase is confirmed by experimental and simulated HRTEM images along the [011] and [012] zone axes. These results provide a fundamental understanding of the IST chalcogenide material for multilevel PRAM.

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