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First-principles Study of Phonons in Structural Phase Change of Ge-Sb-Te Compounds YOUNG-SUN SONG, Pohang University of Science and Technology, JEONGWOO KIM, University of California, MINJAE KIM, SEUNG-HOON JHI, Pohang University of Science and Technology — Ge-Sb-Te (GST) compounds, exhibiting substantial electrical and optical contrast at extremely fast switching modes, have attracted great attention for application as non-volatile memory devices. Despite extensive studies of GST compounds, the underlying mechanism for fast transitions between amorphous and crystalline phases is yet to be revealed. We study the vibrational property of various GST compounds and the role of nitrogen doping on phase-change processes using first-principles calculations. We find that a certain vibrational mode (Eu) plays a crucial role to determine transition temperatures, and that its frequency depends on the amount of Ge in GST. We also find that the nitrogen doping drives crystalline-amorphous transition at low power consumption modes. In addition, we discuss the effect of the spin-orbit coupling on vibration modes, which is known essential for correct description of the electrical property of GST. Our understanding of phonon modes in GST compounds paves the way for the improving the device performance especially in terms of switching speed and operating voltage.

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