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**First-principles Study of Atomic Rearrangement in GeTe-Sb<sub>2</sub>Te<sub>3</sub> Superlattice** YOUNG-SUN SONG, SEUNG-HOON JHI, Pohang Univ of Sci Tech, CNPL TEAM — GeTe-Sb<sub>2</sub>Te<sub>3</sub> chalcogenide superlattices, known as interfacial phase change memories (iPCMs), have been claimed to outperform Ge-Sb-Te-based phase-change materials. Despite its great potential as next-generation non-volatile memory devices, we still lack clear knowledge of the phase change mechanism. According to a recent work, the phase change processes in iPCMs involve two-step atomic rearrangements of Ge-Te layers, but the detailed interatomic features still remain unresolved. In this work, we studied the nature of atomic layer rearrangements in iPCMs using first-principles calculations and the interatomic potential model. We used the climbing image nudged elastic band (CI-NEB) method to obtain the intermediate structures and energies during the rearrangement processes. Applying a simple interatomic potential model to in-between steps, we investigated the interatomic motion during the phase change process. We found that a few selected atomic pairs determine most the energy barrier and also the response to external pressures.

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