Machine Learning Potentials for Phase Change Materials for Electronic Memories

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Phase change materials (PCMs) are chalcogenide alloys exploited in key enabling technologies such as non-volatile electronic memories and neuromorphic computing [1]. In the phase change electronic memory, the two digital states are encoded in the amorphous and crystalline phases of PCMs that feature a large difference in the electrical resistivity. Readout of the memory consists of the measurement of the resistance at low bias while the set/reset processes consist of a fast and reversible transformation between the two phases induced by Joule heating.

Atomistic simulations based on density functional theory (DFT) have provided useful insights on the structural and functional properties of PCMs over the years [1]. However, several key issues for the operation of the devices are presently beyond the reach of DFT simulations. A route to overcome the limitations in system size and time scale and enlarge the scope of DFT methods is the generation of machine learning interatomic potential trained on a DFT database for large scale molecular dynamics simulations. The first application of this approach to PCMs dates to 2012, when we devised a Neural Network interatomic potential (NNP) for GeTe [2] with the scheme proposed by Behler and Parrinello [3]. The NNP was then used to study the crystallization process and the thermal conductivity and aging of the amorphous phase in bulk and in nanowires [4].

In this talk, I will report on the generation of a NNP for the flagship $Ge_2Sb_2Te_5$ ternary alloy [5,6], within the framework implemented in the DeePMD-kit package. The NNP allowed us to perform MD simulations of million-atom models at the length and time scales of the real device to uncover the kinetics of the set process (crystallization of the amorphous phase) at the operation conditions of the memory [7]. Insights on the relaxation times and on heterogeneous dynamics in the supercooled liquid phase of $Ge_2Sb_2Te_5$ will be discussed as well [8].

[1] W. Zhang, R. Mazzarello, M. Wuttig, E. Ma, Nat. Rev. Mater. **4**, 150 (2019).
[2] G. C. Sosso, G. Miceli, S. Caravati, J. Behler, M. Bernasconi, Phys. Rev. B **85**, 174103 (2012).
[3] J. Behler and M. Parrinello, Phys. Rev. Lett. **98**, 146401 (2007).
[4] G. C. Sosso and M. Bernasconi, MRS Bulletin **44**, 705 (2019).
[5] O. Abou El Kheir, L. Bonati, M. Parrinello, M. Bernasconi, npj Comp. Mater. **10**, 33 (2024).
[6] D. Acharya, O. Abou El Kheir, S. Marcorini, M. Bernasconi, Nanoscale **17**, 13828 (2025).
[7] O. Abou El Kheir, M. Bernasconi, Adv. Electr. Mater. e2500110 (2025).
[8] S. Marcorini, R. Pomodoro, O. Abou El Kheir, M. Bernasconi, arXiv:2506.13668 (2025).