ATOMISTIC SIMULATION OF PHASE CHANGE MATERIALS FOR NON-VOLATILE MEMORIES

O. Abou El Kheir[1], D. Dragoni[1], M. Bernasconi[1,*]

[1]Department of Materials Science, University of Milano-Bicocca, Milano, Italy
(*) marco.bernasconi@unimib.it

Phase change chalcogenide alloys are among the most promising materials for in-memory computing and for the emulation of synapses and neurons in neural network devices. These applications rest on a fast and reversible transformation between the amorphous and crystalline phases induced by Joule heating. The large difference in the electrical resistivity between the two phases enable encoding a binary, multilevel or even analogical information if partial crystallization could be controlled. The same features are exploited in phase change electronic memories (PCMs) which already entered the global market as a first example of storage class memories that combine non-volatility with access time close to that of the volatile DRAM. Materials in the same class are also investigated for embedded phase change memories operating at high temperatures for the automotive sector.
In this talk, we will discuss two recent examples on the use of electronic structure calculations to elucidate the relationship between the structure and composition of phase change alloys and their functional properties exploited in the devices. In the first example, we will discuss the results of high throughput DFT calculations aimed at tuning the composition of GeSbTe ternary alloys to raise their crystallization temperature [1]. The second example addresses the effect of confinement on the crystallization kinetics of ultrathin films of Sb which is an example of a monoatomic phase change material [2]. Large scale simulations of Sb in confined geometries have been performed by using an interatomic potential generated by fitting a large DFT database with a neural network method [3].

Keywords
Phase change materials; non-volatile memories; density functional theory; neural network.

Funding
European Union's Horizon 2020 research and innovation program under grant agreement No. 824957, project BeforeHand.

References
[1] O. Abou El Kheir, M. Bernasconi, "High-throughput calculations on the decomposition reactions of off-stoichiometry GeSbTe alloys for embedded memories", Nanomaterials 21, 2382 (2021).
[2] D. Dragoni, J. Behler, M. Bernasconi, "Mechanism of amorphous phase stabilization in ultrathin films of monoatomic phase change material", Nanoscale (2021). DOI: 10.1039/d1nr03432d.
[3] J. Behler, M. Parrinello, "Generalized Neural-Network Representation of High-Dimensional Potential-Energy Surfaces", Phys. Rev. Lett. 98, 146401 (2007).