AB INITIO SIMULATIONS OF PHASE-CHANGE MATERIALS

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Phase-change materials (PCMs) are capable of switching very rapidly and reversibly between the amorphous and crystalline phase at high temperature. Yet, the two phases are stable at room temperature and exhibit pronounced optical and electrical contrast. These unique properties have resulted in applications in rewritable optical devices (CD, DVD, Blu-Ray Disc) and electronic non-volatile random access memories (PC-RAM), where heating is induced by laser irradiation and the Joule effect, respectively.

In this talk, I will present our recent work, based on density functional theory simulations, about the structural, electronic and kinetic properties of the crystalline and amorphous state of selected PCMs.

First I will discuss the structure and the electronic states of crystalline PCMs. I will show that structural transitions and metal-insulator transitions driven by disorder occur in the technologically most important family of PCMs, namely the GeSbTe compounds. Our simulations have enabled us to elucidate the microscopic mechanisms driving both transitions.

Then I will focus on the amorphous state and show that *ab initio* molecular dynamics methods combined with enhanced sampling techniques not only yield realistic models of this state but can also provide important information about relaxation phenomena, which occur on much longer time scales than those accessible by plain *ab initio* simulations.

I will also will present our recent results about crystallization of amorphous GeSbTe and doped Sb_2Te PCMs. I will show that high-temperatures simulations yield crystal growth velocities in good agreement with experimental data. I will discuss the links between the fragility of the supercooled liquid phase of these materials and the ability of the glass to crystallize rapidly at high temperature and yet to be extremely stable at room temperature.

Finally, I will focus on our work about the magnetic properties of GeSbTe doped with magnetic 3*d* impurities, which has shed light on recent experimental work claiming that such doped PCMs exhibit a magnetic contrast between the amorphous and crystalline state.