



Network for Computational Nanotechnology & c-PRIMED Seminar Series

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Friday, May 27th at 10am
 Neil Armstrong Hall of Engineering, Room
 B061

Nanosecond DFT simulations of amorphous-to-crystalline transition

Phase-change (PC) materials are chalcogenide alloys that are ubiquitous in the world of rewritable optical storage media, familiar examples being digital versatile disc (DVD-RW) and Blu-ray Disc. Nanosized bits in a thin polycrystalline layer are switched reversibly and extremely rapidly between amorphous (a) and crystalline (c) states by laser irradiation or resistive heating, and the state can be identified by changes in resistivity or optical properties. The rate-limiting process in PC optical memories is the extremely rapid (nanosecond time scale) crystallization of nanosized amorphous “marks” in a polycrystalline layer. Our knowledge of the amorphous and ordered structures of Ge/Sb/Te and Ag/In/Sb/Te alloys has improved significantly in recent years and has led to plausible pictures for the transition between them. Nevertheless, the simulation of the actual crystallization process is complicated by the need to study large numbers of atoms over time scales that are difficult to attain, even with modern supercomputers. We have performed a series of density functional/ molecular dynamics (DF/MD) simulations on a sample of Ge₂Sb₂Te₅ (GST-225) with 460 atoms. Simulations at 500 K, 600 K, and 700 K have been performed for up to 600 picoseconds in samples where crystallization was promoted by fixing the structure of a crystalline “seed”, and for over 5 ns in four samples at 600 K without constraints. A comparison of the last four simulations shows a striking memory effect where crystallization is favored in an amorphous sample that had previously been crystallized.

Jaakko Akola studied Physics in the Universities of Helsinki and Jyväskylä, Finland, obtaining his Ph.D. at Jyväskylä under Prof. Matti Manninen. He carried out post-doctoral research at the Forschungszentrum Jülich in 2000-2005, and afterwards, worked as senior scientist in the University of Jyväskylä until 2010. He is Associate Professor at the Tampere University of Technology, Finland, where he heads the Materials and Molecular Modeling (M&MM) group. His fields of interest include classical, tight-binding, and density functional simulations of materials, nanoparticles, and biological systems. He is the coordinator of the H2020-NMP project “CritCat” (2016-2019) on rational design of new catalyst materials and Deputy Editor-in-Chief of a new open-access journal *Advances in Physics: X* by the publisher Taylor & Francis.