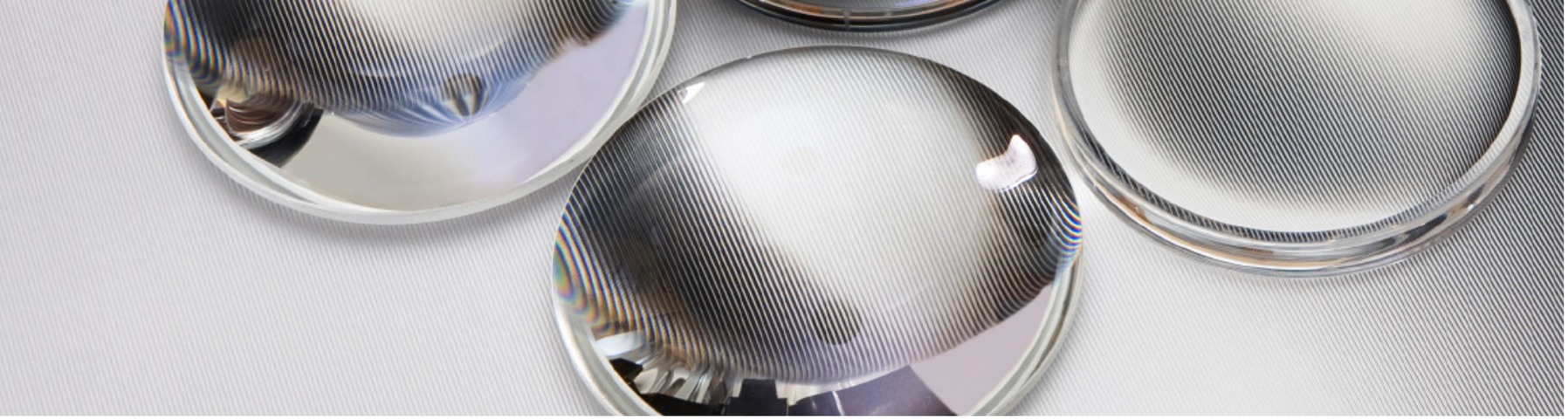


CHALCOGENIDE GLASSES

Drabold models candidates for computer memory

Chalcogenide glasses, compounds based upon the elements sulphur, selenium and tellurium, have been studied extensively for the last few decades. Scientists have examined these compounds both for basic scientific interest in the compounds and because they are preferred materials for technology applications, such as optical recording devices and two novel forms of non-volatile computer memory: "phase change" (PCM) and "conducting bridge" (CBRAM).

"Since the properties of chalcogenide glasses are derived from their structure, knowledge of the structure of these glasses is an essential precursor for further study," said David Drabold, Ph.D., a distinguished professor of physics at Ohio University.

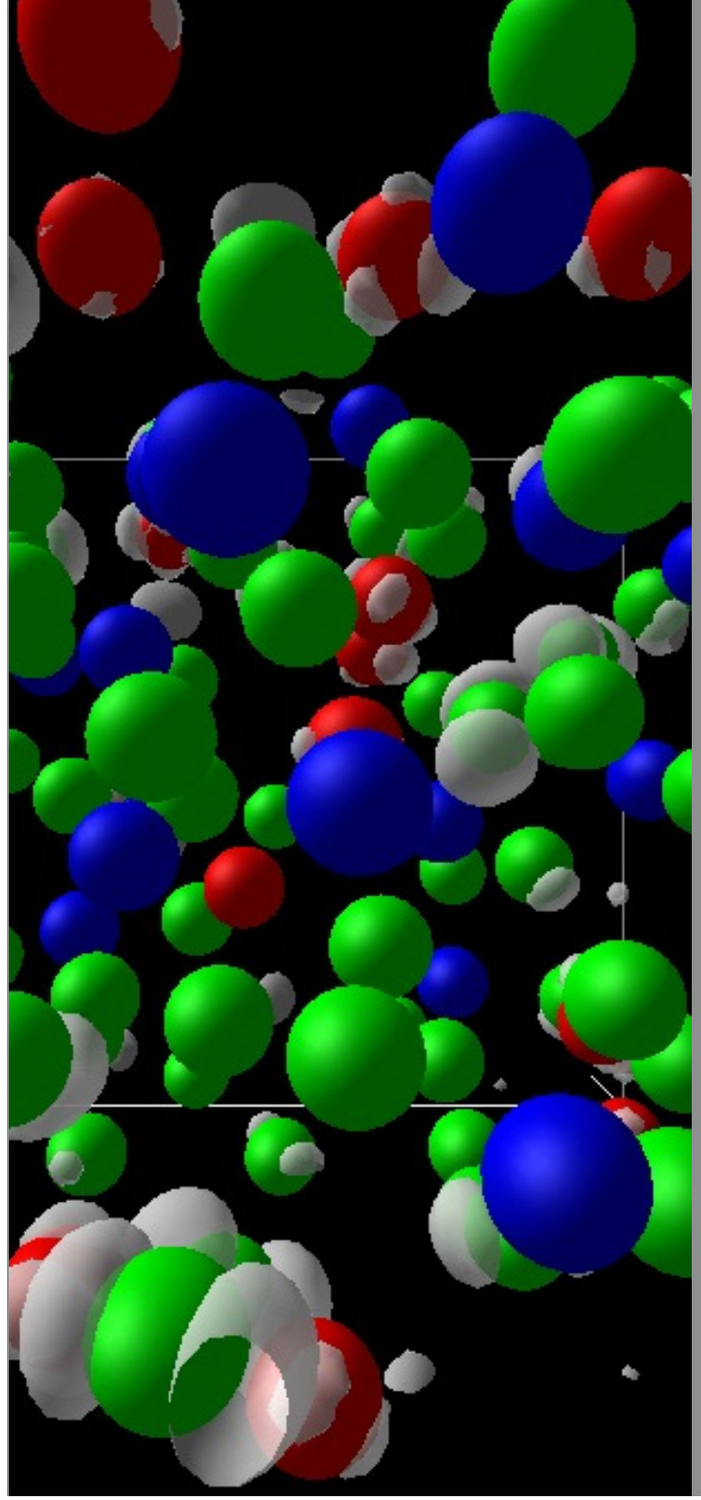
"We use density functional methods to model both PCM and CBRAM materials and work out the key dynamical processes. It's known somewhat empirically that these devices perform very well, but there are many mysteries as to how the devices rapidly switch, such as at the atomistic level. We hope to offer information on how to optimize the materials."

The CBRAM materials are based upon glasses composed of germanium and selenium. When doped with metals like silver or copper, germanium-selenium glasses become solid electrolytes with high ionic conductivities. Under different bias conditions, they possess two stable phases with different electrical conductivities, a contrast that enables their use for information storage.

For PCM materials (also used in DVDs) the contrast is found between the amorphous and crystal phases. Drabold and his research team have directly simulated amorphization and crystallization on extremely fast time scales of ~500 picoseconds (500 trillionths of a second).

"We have employed Ohio Supercomputer Center facilities to explore new materials, previously terra incognita experimentally and theoretically," said Drabold. "It is most unusual to be able to directly simulate phase transitions or ionic diffusion using standard ab initio molecular dynamics. We have a unique opportunity to work out important physical processes of basic interest, and also to provide information of value to applied scientists hoping to optimize their electronic devices."

The chalcogenide glasses work has been carried out in collaboration with Gang Chen, Ph.D., Ohio University assistant professor of physics, and graduate student Binay Prasai. The Vienna Ab Initio Simulation Package (VASP) has been a key tool used for creating the simulations.



Representation of a fully crystallized germanium, selenium, tellurium and silver structure.

Project lead: David Drabold, Ohio University
Research title: Structure and dynamics of chalcogenide glasses
Funding source: National Science Foundation
Web site: http://bit.ly/OSC-RR-Drabold