Simulating Phase Change Materials : how crystal bonding features lead to the formation of a non-Zachariasen glass.

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In the last two decades, Phase Change Materials have emerged as active components of non-volatile memories thanks to their ability to switch extremely rapidly from a conducting crystal to a semiconducting glass. Ab Initio simulations helped understanding the structure and some properties of the glassy phase, like aging, but also led us to reinvestigate the nature of chemical bonding in the crystalline phase.

Using a two electron (pair density) formalism, we develop a two-dimensional map[1] based on a quantum-topological description of electron sharing and electron transfer in binary solids. This map intuitively identifies the fundamental nature of ionic, metallic, and covalent bonding in a range of elements and binary materials. More interestingly, it highlights a distinct region where phase change materials are found and for which bonding has been qualified as 'metavalent'[2]. This metavalent region of the map encompasses other compounds with enhanced properties, such as high thermoelectric performance or photovoltaic efficiency[3]. We illustrate metavalent bonding for lead chalcogenides and V-VI compounds, and the transition between covalent and metavalent regions of the map is described [4].

Interestingly, we show that it is possible to transform regular covalent bonds metavalent through excitation, which can explain the ovonic threshold switching behavior[5] of some chalcogenide glasses, or sub-picosecond laser induced phase transitions[6].

Finally, we show that metavalent bonding does not subsist is the glassy state of phase change materials, in which bonding is essentially covalent with 'regular' associated properties. This is different from many glasses (so-called 'Zachariasen' glasses) in which local atomic ordering and electronic properties are similar between the glass and the amorphous phase.

References

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