**Role of nuclei in phase-change materials**

The most commonly studied phase-change material is Ge$_2$Sb$_2$Te$_5$ (GST). Simulations show that unstable nuclei in the amorphous phase contain ABAB squares and cubes that resemble those seen in crystals. Crystallization takes several nanoseconds.

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### Role of nuclei in phase-change materials

**Unstable nuclei at 600 K**

**Crystallization trajectory**

- **Crystallization**
  - 0.87 ns
  - 1.15 ns
  - 2.75 ns

**ABAB rings**

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**Graph:** C. Bickel/

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**References**


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**SCIENCE**

**Speeding up crystallization**

Chemical insights from simulations help to design a phase-change material that can crystallize in less than a nanosecond.

By J. Akola and R. O. Jones

Phase-change materials (PCMs) form the basis of many modern optical-storage media (such as DVDs) and promise to yield faster, more stable random-access memory (RAM) devices for computers. All of these devices are based on the fast and reversible crystallization of amorphous bits in thin polycrystalline alloy layers, with crystallization being the time-limiting stage. Optimization of the alloy composition for faster crystallization is a major challenge in speeding up this process. On page 1423 of this issue, Rao et al. (1) take full advantage of atomic-level knowledge of the structure and crystallization properties of PCMs from simulations to develop a new alloy with greatly reduced nucleation times and demonstrate subnanosecond crystallization in a PCM device based on this alloy.

The Materials Genome Initiative was set up in 2011 by the U.S. government with the mission of accelerating the discovery of advanced materials (for example, for batteries and photovoltaic devices) and thereby lowering the cost and time to market by at least 50%. Computational tools play a crucial role in this endeavor alongside experiments and digital data, and the screening of many compounds and vast amounts of data to isolate those with the desired properties can complement traditional trial-and-error experiments. In contrast to these data-intensive approaches, Rao et al. surveyed the results of computer simulations (particularly using density functional theory) and experimental studies of PCMs performed over the past decade and used the resulting chemical insight to identify the properties required for rapid crystallization.

Most PCMs used in optical storage are alloys containing antimony (Sb) and tellurium (Te), both of which tend to crystallize spontaneously in the amorphous state. Other elements often used in PCMs are germanium (Ge), silver, and indium. The most-widely studied PCM alloy is germanium antimony telluride (Ge$_2$Sb$_2$Te$_5$ or GST), and scientists have found it difficult to improve upon the speed, stability, and cyclability of its crystallization properties.

Numerous simulations of GST have shown that amorphous and crystalline GST contains structural units referred to as ABAB rings (where A is Ge or Sb and B is Te) (2–4), suggesting that they act as nuclei for crystallization (see the figure). Ge atoms occur in both octahedral and tetrahedral configurations; the latter are associated with Ge–Ge bonds that are unfavorable to crystallization (2, 5). Small crystallites (nuclei) appear and disappear during crystallization at temperatures below the melting point, implying diffusion and bond-breaking, both of which appear to hamper crystallization (6, 7). Nucleation is inherently unpredictable, and crystallization takes several nanoseconds, even in computer simulations (7).

In their search for a superior PCM, Rao et al. sought materials that do not contain Ge but nevertheless form robust ABAB rings. The authors considered telluride alloys, including all transition metals and noble metal elements except for gold. On the basis of chemical considerations and simulations, they predicted that adding small amounts of the transition metal scandium (Sc) to antimony telluride (Sb$_2$Te$_5$) should yield a PCM with superior properties.

In subsequent experiments, the authors found that the optimal alloy was Sc$_2$Sb$_2$Te$_5$, which has strong Sc–Te bonds and many of the favorable properties of GST. Density functional calculations revealed that the octahedral structures associated with Sc are much more robust than those in GST, and experiments with a PCM device using this new material showed that subnanosecond crystallization times are attainable. Rapid crystallization is an inherent property of the material, such that no pretreatment of the sample, for example, with a weak electric field (6), is necessary. Importantly for RAM, the new material’s amorphous phase has a similar thermal stability as GST, and the material can be cycled over 10$^7$ times without a notable resistivity change.

Density functional calculations have experienced dramatic growth in recent decades and provide a description of materials properties based on the electronic structure alone, rather than on experimental measurements. Despite their computational demands and the resulting restrictions to short simulations on small samples, they can provide valuable insight into underlying physical phenomena. Rao et al. show how this knowledge can be used to design materials with much improved properties and demonstrate the strength of the rational materials design approach.

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