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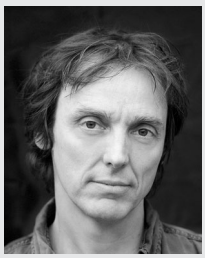
MATERIAL WITNESS

# Searching under pressure



Philip Ball

Diamonds are forever, but that's a thermodynamic peculiarity. The brilliant gems in wedding rings and crown jewels are only metastable with respect to graphitic forms of carbon. Diamonds show not only how valuable, practically and economically, metastable materials can be but also how robust, if the kinetic barriers protecting their transformation to the ground-state polymorph are high enough.

The first synthesis of diamond in the 1950s roughly recapitulated the extreme conditions of temperature and pressure under which they form in the natural environment. Producing such non-ambient conditions is now rather routine, not least by means of diamonds themselves as the teeth of diamond-anvil cells. It was by using such methods, for example, that a new high-pressure phase of boron was recently produced, which has a hardness comparable to that of cubic boron nitride and, like diamond, is quenchable to ambient conditions[1].

But in searching for other potentially useful metastable phases it is not easy to know what to look for, because their prediction is complicated. Techniques for predicting high-pressure crystal structures[2] are typically computationally expensive. Meanwhile, machine-learning algorithms exist for predicting stable materials by interpolation from large databases, supported by density-functional calculations of some key properties based on the crystal structures[3]. But these databases (sometimes called a 'materials genome') are restricted to ambient conditions — in fact, generally to zero temperature and pressure.

Amsler et al. have now developed a method that allows the information in such databases to be extrapolated to non-ambient conditions so as to identify potential metastable high-pressure phases[4]. They point out that it is often under such conditions that materials may develop useful properties such as hardness, high energy density or high coordination that could be exploited if a phase is quenchable.

The technique rests on a rather crude but nonetheless workable linear extrapolation of the enthalpy of ambient phases to high pressure. In several test cases for known high-pressure phases, the researchers found that phase boundaries are not much better predicted by more sophisticated enthalpy calculations — for example, including second-order, nonlinear terms.

Because the method is computationally cheap, it can be applied to the many thousands of materials represented in databases, supplying good statistics about performance. For binary compounds, about 80% of the phases that have been shown to be stable experimentally are predicted to be so by extrapolation from ambient-pressure data using this method. What is more, around 60% of the binary phases that are metastable at ambient conditions become ground states at non-ambient conditions. Those two things are not obviously connected — glassy phases, for example, are not generally ground states under any conditions. An implication might be that when metastable phases are found experimentally in materials synthesis, there is a good chance that they might be quenched forms of states actually produced under more extreme local conditions due to fluctuations in, say, pressure. In such ways, methods like this might not just assist materials discovery but also offer insights into the broad features of the multidimensional thermodynamic landscape that govern material stability. ❐

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