

August 2006

News and Views

PHILIP BALL

Material Witness: Dynamic days

doi:10.1038/nmat1704

The history of materials science over the past 50 years has been about mastery of structure. Discuss, as an examiner might say. In other words, consider this not as a statement of supposed fact but a springboard for debate.

I am probably not alone in being in thrall to notions of structure, and bedazzled by today's command of it. True, it is still not possible to predict the atomic-scale structure even of a relatively simple material from stoichiometry alone — a shortcoming in crystal engineering that Nature once provocatively pronounced a scandal. But from DNA lattices to biomimetic composites to nanoporous solids, the control of structure now on display is staggering.

Yet that is just one aspect of the objective of obtaining materials properties by design. In particular, I have been reminded by Ahmed Zewail at Caltech of the other, often neglected, facet of molecular-scale function: dynamics.

Traditionally, materials scientists have tended to feel less need to consider dynamical behaviour than chemists. After all, many traditional materials are meant to be relatively inert, to perform their role mechanically. There are, of course, plenty of properties that do depend on dynamical behaviour in 'traditional' fields: defect migration in semiconductors, say, or crystal growth, or crack propagation. But you see the point.

As the functions of materials diversify, however, the problem of not only understanding but also controlling dynamics, in terms of the exploration of an energy landscape, becomes ever more urgent. This is particularly evident for materials that interact with biological systems, as no one now doubts that biomolecular interactions are deeply affected by dynamics.

In drug design, for example, it is often not enough to look for a good fit with a protein's binding site in terms of the static placement of favourably interacting chemical groups. The trajectory of the binding event on the energy landscape can be crucial. Now factor that into the suggestion by Matthew Tirrell at the University of California at Santa Barbara that "modern biomaterials science is largely devoted to display of biological signals on synthetic material surfaces", and you begin to see that mastery of dynamics may emerge as one of the next big challenges in materials science.

Or take the question from George Whitesides at Harvard: "How do I plug my computer into my brain?" In other words, how to interface organic tissue and silicon? Or consider his question of how to make a molecule "so that it polymerizes into a moldable solid that in turn is a semiconductor with high hole mobility". If such properties depend on

controlling polymer conformation, then that may be at least partly a dynamical problem, as any protein chemist will confirm. But understanding molecular-scale dynamics is an enormous challenge, not least because it may involve such a wide range of timescales. We have barely scratched the surface.