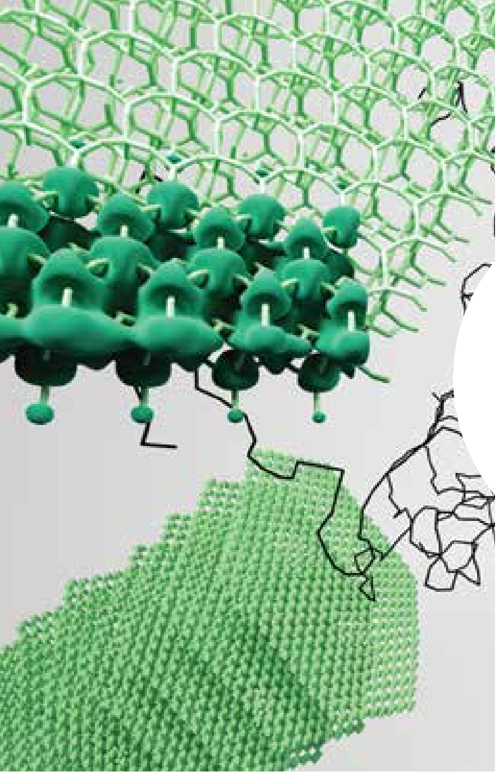

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A NEW FRONTIER FOR MATERIAL SCIENCE: DESIGNING NANOCOMPOSITES IN A VIRTUAL LABORATORY

Nanocomposites are a new frontier in materials science. Existing nanocomposite materials are highly prized due to their unique properties. From the discovery of new medicines, through helping bones to heal faster, to uses in the car industry, nanocomposites have applications in lots of areas of our daily lives.

Creating new nanocomposite materials with a set of desired properties is challenging. Traditionally, it has been very difficult to create new materials, as these would have to be created by hand using a trial-and-error process. Not being able to predict the properties of the materials meant that it was necessary to create many of these before just one useful one was found.

Researchers at UCL have used ARCHER to create a virtual laboratory to aid in the understanding of nanocomposite materials, so new ones can be designed. The researchers use multi-scale modelling to predict the properties of a nanocomposite from its atomic make-up. In this case, it was used to discover previously unknown information about the structure of clay-polymer nanocomposites. This allowed them to understand why these materials have their properties. The principles underlying the virtual laboratory are applicable to the entire field of nanocomposites, so could have a huge impact on studies in this area. The tools developed here are, in fact, already being applied to drug discovery, seeing how new drugs interact with their targets.

UCL

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MAPPER

الصندوق القطري لرعاية البحث العلمي
Qatar National Research Fund

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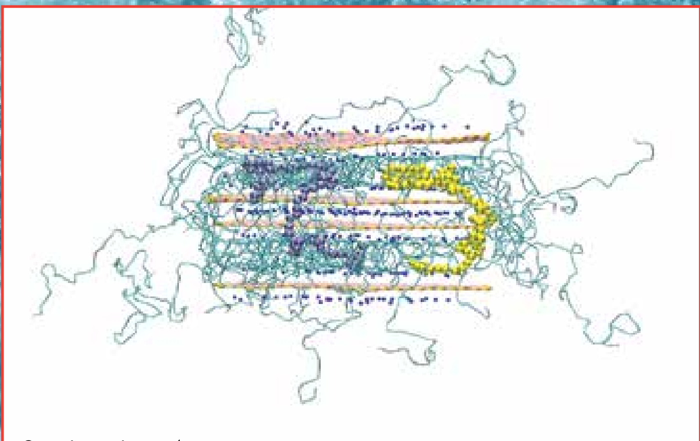
Nanocomposites – a new frontier

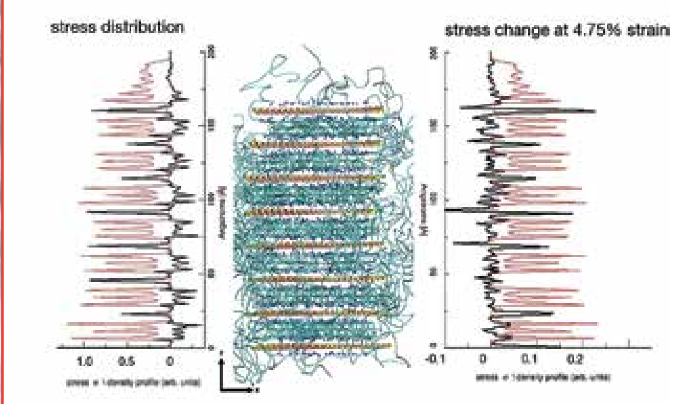
Nanocomposites are materials which contain nanoparticles. These are contained in a matrix material, and work to strengthen or change the matrix's properties. For example, adding carbon nanotubes to bone cells causes bone to heal faster. Nanocomposites can be man-made but also occur naturally in materials such as abalone shells, bone, and clay.

Both natural and man-made nanocomposites are used throughout industry. Carbon fibre, a material used extensively within the automotive industry, is a nanocomposite material. Other nanocomposites are also used in vehicle manufacture. In fact, one of the first commercial applications of clay-polymer nanocomposites was created by Toyota, who used clay to reinforce nylon in their vehicles. Both of these materials have interesting and useful properties – they are extremely strong despite their low densities. Graphene is also a nanomaterial, and one that has shown great promise in many potential applications. However, progress has been stalled by difficulties in understanding how we can best utilize graphene's properties and manufacture useful materials.

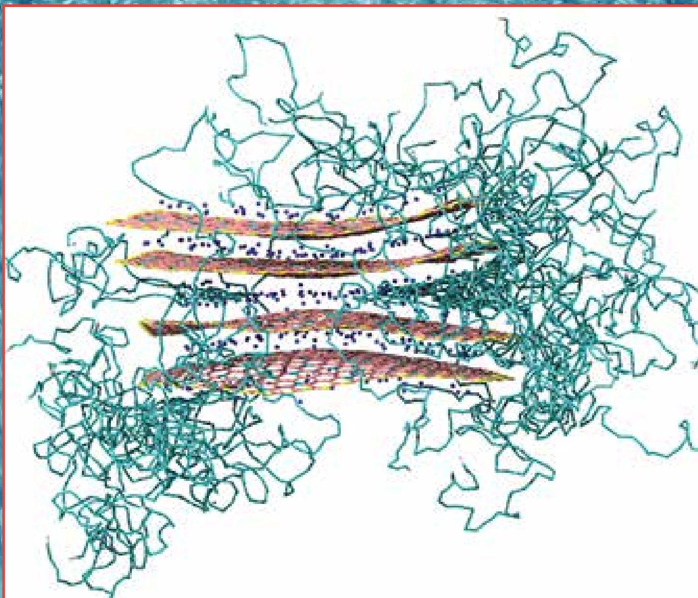
Nanocomposites are useful as their physical and chemical properties often differ wildly from those of their components. As the particle size of an element gets smaller, its behaviour changes and its properties become size-dependent. At nanoscale, normally unreactive elements such as gold become highly reactive. Melting points, conductivity, fluorescence, and magnetic properties may all change.



Crossing polymers[1]



Stress strain breakdown[1]



Initial intercalation crop[1]

The Virtual Laboratory

Searching for new nanocomposite materials is not easy. Only a few have been created, despite great interest in the field. The ability to custom-design materials exactly is extremely attractive, but there are many obstacles. First, until very recently, the reasons why nanomaterials have their properties, and why they differ from their components, was not fully understood. Secondly, it can take time to create new nanocomposites; often this involves grinding the nanoparticle, adding them to a matrix, and then testing the properties of the material. It may take many tries until a useful material is created.

Research using ARCHER has created the first step towards a 'virtual laboratory', where nanocomposite materials can be designed. The 'virtual lab', which uses a job automation tool called FabSim[2], makes finding new nanocomposites much easier. This is done simply by inputting the molecular structure, chemical composition, and processing conditions. The 'lab' then uses multi-scale modelling to simulate the properties of new materials based on this. Here, this method was used to discover the exact reason behind the properties of clay-polymer nanocomposites. However, in future, it could be used to discover and understand a range of different nanocomposite materials.

Why Clays?

The virtual lab has been used to study clay-polymer nanocomposites - the same type created by Toyota. Clays occur naturally as tactoids – flat, elongated plates - anywhere from just a few, to as many as one thousand stacked sheets. These sheets are tightly packed together, but individual sheets may sometimes break off under certain conditions. The properties of a clay–polymer nanocomposite are thought to depend on how, and to what extent, the tactoids separate.

The simulations showed, for the first time, exactly how the polymer matrix interacts with the clay tactoids. It was discovered that the polymers move between the stacked clay sheets and, in some cases, this causes the stacks to break apart[3]. The stacks can break apart in different ways, creating materials with different properties. The simulations also allowed the clay-polymer interactions to be studied over a long timescale. This is one of the unique selling points of simulations, as this would not have otherwise been possible. From these simulations, the researchers were able to see how the clay-polymer complexes arranged themselves into stacks over time. These stacks had different properties depending on their precise makeup.

The virtual lab's predictions are already in use, improving the construction of new nanocomposite materials.

Why ARCHER?

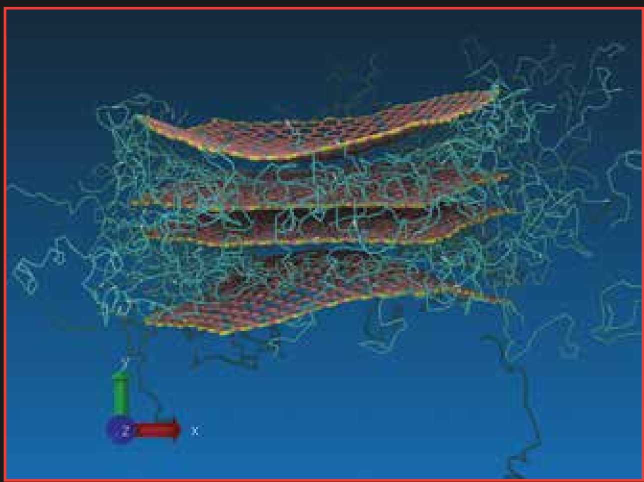
The virtual lab research was not only conducted on ARCHER, but ARCHER offered positives other machines did not. ARCHER was chosen for a number of reasons, including its performance, ease-of-use, reliability and level of support. It is able to run the code used here, LAMMPS, very efficiently, showing better scalability than a number of other machines. The scheduling policies on ARCHER also allowed the researchers to run quick, small parametrization runs, and so were able to quickly calculate the parameters needed for the large-scale simulations. The better scalability of ARCHER also meant that these large runs completed faster than they would have on other machines.

Results

The major scientific outcome of this work was the construction of a 'virtual lab' for materials discovery[4]. Its key feature is that it is able to predict the properties of materials just from their atomic makeup. Here, it was used to model the process of polymers entering between layers of clay, to eventually form a new composite material.

This has the potential to be transformational for the nanocomposite field. In the short term, it can speed scientific discovery and understanding in the field. In the longer term, eliminating costly and time-consuming trial-and-error will improve materials science. This should enable materials scientists and engineers to search systematically for desirable nanocomposites.

The lab has a variety of potential applications. Tools developed are currently being used to predict the properties of potential new drug compounds, by investigating how molecules bind to target receptors. This modification shows the potential of this research for more than just clay-polymers. Thus, this research could have significant impact due to the wide variety of potential uses for nanocomposites.



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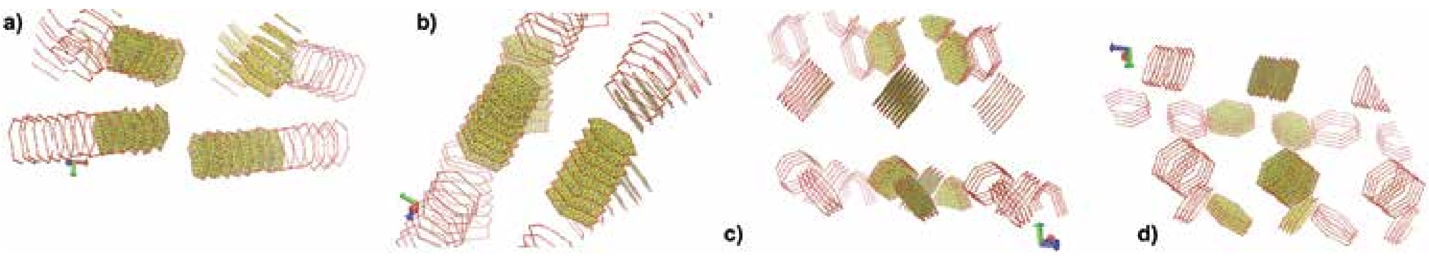

www.archer.ac.uk

About ARCHER

ARCHER is the UK National Supercomputing Service. The service is provided to the UK research community by EPSRC, UoE HPCx Ltd and its subcontractors: EPCC and STFC's Daresbury Laboratory, and by Cray Inc. The Computational Science and Engineering (CSE) partners provide expertise to support the UK research community in the use of ARCHER. The ARCHER CSE partners are EPSRC and EPCC at the University of Edinburgh.

The eCSE Programme

The Embedded CSE (eCSE) programme provides funding to the ARCHER user community to develop software in a sustainable manner to run on ARCHER. Funding enables the employment of a researcher or code developer to work specifically on the relevant software to enable new features or improve the performance of the code.

The Case Study Series

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