[subject category: Materials]

SUPERCOMPUTER DETECTS CLAY'S NANOSCALE WOBBLE

Clays are remarkable naturally occurring minerals that are used for everything from pottery to catalysts. However, despite their ubiquity and importance, the way that the atomic-scale structure of clay influences its behaviour is poorly understood.

Now, researchers at University College London have used supercomputers to construct a model of how clay behaves at the level of its constituent atoms – and have discovered that it possesses an inherent, nano-scale wobble that accounts for many of its key characteristics.

Clays are composed of millions of tiny discs called platelets that are aligned in sheets that are themselves stacked up in layers. "We are interested in understanding how materials work at the molecular level so that we can begin to control what we can do with them," says Professor Peter Coveney of UCL. "But with clays the individual platelets are too small to measure their properties accurately."

To get around this the UCL researchers have constructed huge computer simulations of millions of atoms of the elements that make up clay – approaching the size of a single platelet, which is typically about 1 nanometre (billionth of a millimetre) thick and between 100 nm and 1000 nm across.

"The only way to achieve a simulation of this complexity is to use a supercomputer of hundreds or thousands of processors linked together," Professor Coveney says. "By doing this we have discovered phenomena within clay that people had not expected. In particular at a molecular scale the layered sheets are in a constant state of motion caused by thermal energy. They are continuously undulating, and not rigid as was previously thought. Intriguingly this motion accounts for many of the properties of the material that we can measure, such as its elasticity."

This type of information will be important when developing new uses for clays, Professor Coveney says.

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IMAGE CAPTION: Atomic lasagne…layers of atoms in clay are continuously undulating at the nanoscale


450 Å