Concrete **achievements**

Expert materials scientists **Professors Gaurav Sant** and **Mathieu Bauchy** and **Dr Aditya Kumar** explain their ambitious work towards increasing the sustainability of cement production, and the diverse scientific backgrounds that led them to this important research endeavour

Could you provide an insight into your individual backgrounds, and the research being conducted by the Civil Engineering Materials Group at the University of California, Los Angeles (UCLA)?

GS: I was recruited by UCLA in 2010 to build a programme in civil engineering materials. I've been working for three years with Dr Kumar, whose background is in materials science. Professor Bauchy joined the faculty and the Group in 2014. Our backgrounds are diverse – Professor Bauchy is a physicist, whereas I am a civil engineer – which means that although we both work on the materials science of cementitious materials our areas of expertise are quite different. Our main focus is on cements, concretes, glasses and ceramics, ie. materials that are used in a wide variety of industries and which significantly impact our quality of life. We want to develop better versions of these materials, increasing their performance and efficiency as well as reducing their carbon and energy-use impact.

MB: My background is in physics and chemistry, not civil engineering, but I'm interested in the materials that are relevant to this field. Often, materials research is considered something of a trite subject for pure physicists, but I find it exciting to look at materials that are relevant for industry and our society from a physics point of view, and apply novel mathematical theory to help devise solutions.

The Group has a joint expertise in glasses and cementitious materials. From smartphone screens to bridges, what are the synergies between these fields?

MB: Both cement and glass are composed of similar constituents: oxygen, silicon, aluminium, calcium and sodium, some of the most available elements on earth. This means that these materials can be produced cheaply, using abundant raw materials. It's also interesting to note that both glass and the products that form when cement and water react with each other (ie. calcium silicate hydrate) have non-crystalline structures. These two industries are very intensive in terms of carbon dioxide emissions, a factor that we would like to tackle in both cases. The properties that are of interest when designing a new cement or glass are also similar – so we are naturally asking a lot of the same questions, and seeking similar answers for both materials.

Reflecting on the work conducted by the team as a whole, what have been some of its key results? How might this work impact industry and the environment?

GS&AK: In general, we don't pursue questions that have a short-term impact, for a simple reason: if an issue can be realised quickly, then industry alone can address these topics. We're more interested in technologies that could be making a difference in five or 10 years' time. That's not to say that our work doesn't have an impact on industry; we have been actively involved with filing patents and other activities that generate a lot of interest in this area. Our work with limestone and fly ash, similarly, is really helping industry move towards new formulations and better use of materials. When we talk about real impact, we try to address that at a number of levels: not only building a bridge, for example, but improving the performance

factors of that bridge and its lifespan, as well as its carbon footprint, holistically.

How and why is the Group using atomistic simulations, validated by experiments, to advance glasses and infrastructure materials?

MB: In this Group we emphasise a marriage of analytics and simulation, especially at an atomic scale. This seeks to specifically bridge experimental and computational studies, to complement and inspire each other – rather than work at distinct levels, and at cross-purposes. Obviously simulations cannot replace experiments, but once we validate the outcome of a simulation with experiments and the interpretations therein, simulations are a very effective means of modulating, and examining the influences of chemical composition and process parameters on material performance.

Where does the Group aim to concentrate its research efforts in the coming years?

GS&AK: We've made good progress – but it's also safe to say that there is a really long way to go, so in that sense we're in no doubt about our future plans. At the same time, however, there are opportunities to expand our work into biological materials, and those for energy applications (see Figure 3), since many of these materials share characteristics with cement, the calcium silicate hydrates and glass, ie. having complex and nanoscale porosity, being susceptible to degradation and the need for continuous performance improvement.

Cementing the future

In the near future, restrictions placed on CO_2 emissions and penalties therein stand to limit the use of cement-based building materials – but scientists at the University of California, Los Angeles are working hard to ensure that this valuable material remains sustainable, both environmentally and financially, for use in construction

CEMENT IS A material that has become the linchpin of an industry; its massive utility and versatility have made it ubiquitous in modern construction. Being relatively cheap to produce and based on abundant raw components, it has come to be used in applications that no other material could accommodate – and has also given rise to comparably popular mixtures that rely on it, including concrete. Because the use of cement is so pervasive, it is hard to believe that this common and even banal material poses a potent threat to the environment; the production of cement involves heating calcium carbonate to make lime, but this process also releases significant amounts of carbon dioxide (CO_2). In fact, through the production process, for every kilogram of cement produced 900g of CO_2 is released into the atmosphere.

This is an immediately alarming ratio – but perhaps even more striking is the fact that the production of cement may contribute as much as 9 per cent of total anthropogenic CO_2 emissions. Figures like these are worrying for the planet, and they are also bad news for industry and communities everywhere; reducing the production of cement, and the concrete that it is a component of, would mean reduced infrastructure development, far fewer opportunities to build low-cost housing (especially in developing countries), and fewer opportunities to sell concrete and construction services as well. With internationally-agreed emission targets already in place however, cutbacks seem inevitable – and solutions to more efficiently produce and utilise cement are urgently needed.

CHANGING INDUSTRY

There are a number of possible answers to this problem that vary in complexity – but the simplest and most straightforward involve devising more durable forms of the material so that less is needed to fulfil construction goals, and finding new ways of producing cement that do not rely so heavily on decarbonating limestone. If a cement with both of these qualities were to be developed, it could not only affect a sea-change in the carbon sustainability of the industry, but also – if it could be offered at a comparable price – allow for savings that would apply to all stakeholders. The rewards for solving this riddle, therefore, are as significant as the challenge that its solution poses for a material which is used at the scale of > 3.5 billion tonnes, annually.

One group of materials scientists at the University of California, Los Angeles (UCLA) has risen to this challenge. "It is the chemical building blocks of cement (and concrete) that really dictate its performance; if you can alter those, you can optimise and manipulate the material towards its final application," explains Professor Gaurav Sant, field-chair of the University's Civil Engineering Materials Programme. Using experimental methods extended with numerical simulations, UCLA's Civil Engineering Materials Group aims to examine materials at a fundamental level – working not only with cement, but also with other industrially-relevant products like glass, and reapplying lessons learnt between the different materials. Professor Mathieu Bauchy, an expert on the subjects of glass and cement, comments: "These are old and well-established industries with a lot of empirical knowledge accumulated over time. If you want to make an advance in either, then you need to introduce a new point of view and an approach that has not been thought of before".

FROM SMARTPHONES TO CONSTRUCTION SITES

Glass and cement may not seem immediately similar but in fact they share many common features, and it is through the investigation of these shared features that the Group hopes to

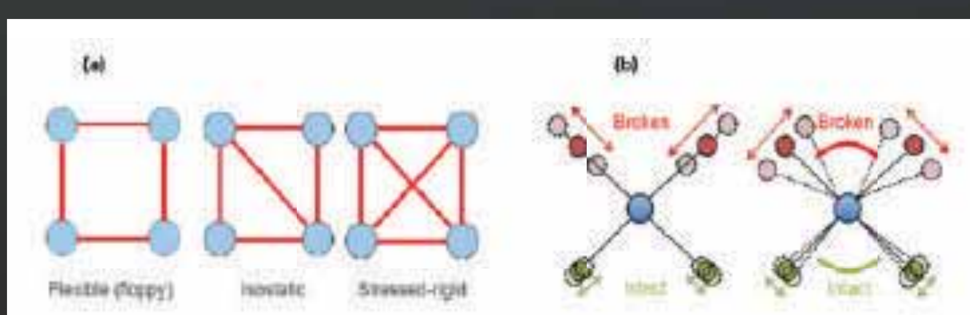

Figure 1. (a) The rigidity states of an atomic network, (b) An illustration of the methodology used within the scope of rigidity theory to compute the number of intact constraints through molecular dynamics simulations.

INTELLIGENCE

CIVIL ENGINEERING MATERIALS GROUP

OBJECTIVES

To comprehensively elucidate structure-property relations for materials of civil engineering relevance, namely cement, glass and concrete.

KEY COLLABORATORS

Professor Jacob Israelachvili, University of California, Santa Barbara, USA • **Professor Pietro Lura**, Empa, Switzerland • **Dr Jeffrey W Bullard**, National Institute of Standards and Technology (NIST), USA • **Professor Narayanan Neithalath**, Arizona State University, USA • **Professor Maria Juenger**, University of Texas, Austin, USA • **Professor Normand Mousseau**, Université de Montréal, Canada

PARTNERS

University of California, **Santa Barbara** • **Empa** • **NIST** • **Arizona State University** • **University of Texas**, Austin • **Université de Montréal**

FUNDING

National Science Foundation • Federal Highway Administration (FHWA) • US Department of Energy • California Energy Commission • Private Industrial Sponsors

CONTACT

Professors Gaurav N Sant and **Mathieu Bauchy**

Laboratory for the Chemistry of Construction Materials (LC[2])
5731 Boelter Hall
Department of Civil and Environmental Engineering
University of California, Los Angeles (UCLA)
California 90095-1593, USA

T +1 310 206 3084, +1 310 825 9991
E gsant@ucla.edu, bauchy@ucla.edu

www.lcc-ucla.com

www.mathieu.bauchy.com

PROFESSOR GAURAV N SANT is an assistant professor and holder of the Edward K and Linda L Rice Endowed Chair in Materials Science in the Department of Civil and Environmental Engineering and Member of the California Nanosystems Institute at UCLA. He earned his PhD (2009) in Civil Engineering from Purdue University.

PROFESSOR MATHIEU BAUCHY is an assistant professor in the Department of Civil and Environmental Engineering at UCLA. He earned his Bachelors (2007) and Masters (2009) in Physics from Ecole Normale Supérieure, Cachan, France, and his PhD (2012) in Condensed Matter from the Université Pierre et Marie Curie, Paris, France.

DR ADITYA KUMAR is a project scientist in the Department of Civil and Environmental Engineering at UCLA. He earned his PhD (2011) in Materials Science from the Swiss Federal Institute of Technology, Lausanne (EPFL), after which he moved to UCLA.

suggest innovative and more efficient routes for industry. A prominent example of this has been the work Bauchy and his colleagues have undertaken towards applying rigidity theory to concrete. Rigidity theory is a logical framework with which the properties of a finished glass can be predicted, based only on their atomic-scale structure. It was this theory that allowed engineers at Corning® Inc. to discover their famous Gorilla® Glass product, a tough glass which is today used for the screens of most smartphones and tablets.

Like glass, an important part of the functionality of concrete is in its toughness; as Bauchy explains: "The strength of the material matters as much for a bridge as it does for the screen of a smartphone". By reapplying rigidity theory from glass to cement, therefore, the UCLA team is working towards elucidating compositions of silicate-materials, ie. glass, cement, concrete and beyond that would have superior qualities. When typical ordinary portland cement (OPC) powder is mixed with water, the resulting paste is composed of a calcium silicate hydrate. As one example, rigidity theory allows the scientists to look at the atoms involved as joints connected together by chemical bonds or rods. Optimising the qualities of this lattice has a big impact on the toughness of the final product – just as was the case with Gorilla® Glass. This is one example of how a better understanding of cement, concrete and glasses would enable the development of high-performance materials for civil engineering.

STRENGTH IN SUBSTITUTION

Sant and his colleagues tweak the chemical makeup of their cement mixture in a simple but effective way: by substituting portions of the cement in the mixture with compatible materials that have a lower carbon impact, such as limestone, clays and coal-combustion

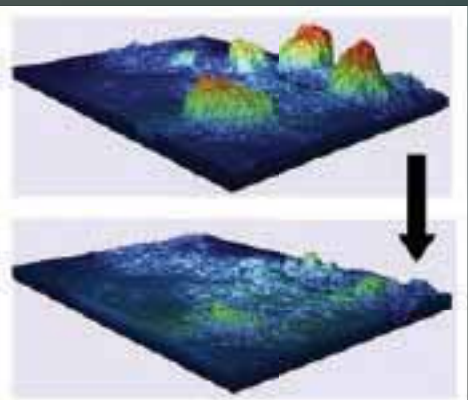

Figure 2. An illustration of calcium silicate (Ca_3SiO_5) particulates as visualised using vertical scanning interferometry. Upon solvent contact, reactions at interfaces solid-solution interfaces (ie. dissolution, precipitation, corrosion) can be tracked by measuring the decrease in particle/surface height over time (ie. from the top-to-bottom image). In the direction of the arrow, the particle height receded several microns over a period of hours on contact with water. Such analytics are enabling cutting-edge measurements of interfacial reaction processes at nanoscale resolution (0.1 nm), in real time.

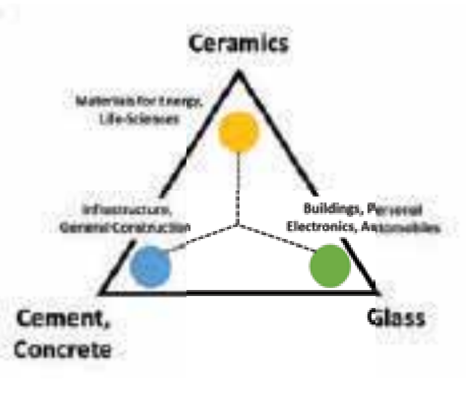

Figure 3. A chart showing the material families and industries impacted by the Group's research within the scope of materials science in civil engineering, and beyond.

residues, eg. fly ash. This is challenging work, particularly because these and similar materials have been used as cement components for a long time, and each poses its own problems. The groundbreaking element of the UCLA scientists' work is their use of nanoscale analytics, (Figure 2) and rigidity theory (Figure 1) to seek optimal 'cementing' compositions, and balance these materials in a way that was never before possible. This breakthrough opens up the possibility of discovering new, more efficient mixtures without costly trial and error.

One of the factors that helps the Group to work so efficiently is the emphasis that they place on computer simulations to extend and expand their experimental results. Faster and cheaper than experimentation, simulations open up a level of detail that would otherwise be inaccessible, and can also be used to optimise experiments before they are performed; and rigorously explain experimental observations. Furthering investigations in this order is what allows the Group to examine cementitious materials in a way that was previously impossible, and to unravel mysteries that other teams have been examining for decades – such as the question of how limestone behaves in cement.

APPLICATION

Working in an area so closely tied with industry, there is always the danger that valuable work could fail to find application without the proper relationships and communication between academics and professionals – but far from considering this as a danger, Sant and his colleagues see it as one of the Group's main strengths. "We really understand the practical end of the business – we offer to solve practical, industrial-scale problems with fundamental science, which is often at difference with how civil engineering materials research is typically approached," he opines. Certainly, despite their short history, the Group has expanded rapidly in size – it now includes two professors, a project scientist, four postdoctoral scholars, nine PhD students and several visiting researchers – and they have already made a considerable impact on practice in the industry and established themselves as leaders in the field. In the future, it is likely that their innovative work will only further cement this enviable position.