

Editorial

Seishi Goto

Professor Emeritus, Yamaguchi University, Japan

People want to understand the nature of materials; however, to do this one has to consider all of the individual levels (atomic, nano, micro and macroscopic). For this computer science becomes a very useful, powerful tool, especially for problems that are not always easy to resolve using an experiment. A computer can easily calculate a big computation, so it sometimes becomes like a black box, in which someone inputs something and can get some results. It is very important for a report to have traceability, but the results are often isolated from interpretation. This means that knowledge increases but understanding does not increase. We have to resolve this problem.

In this issue, the first two papers are related to computer simulation. Zhou *et al.* (2016) used molecular dynamics (MD) simulations based on first-principle calculations, and applied a high-temperature annealing method to build the amorphous structure of calcium–silicate–hydrate (C–S–H). Then the bulk modulus, shear modulus of C–S–H gel and high- and low-density C–S–H, and also the bulk modulus, shear modulus, elastic modulus and Poisson's ratio of cement paste were calculated using the MD method. The paper by Jingjing *et al.* (2016) also uses computer simulations. The nanoindentation procedure were simulated with the combination of the van der Waals function and the peridynamic force function with an assumption of discrete particles of high- and low-density C–S–H. The peridynamics theory is based on the force interaction of a non-local model instead of the spatial partial differential equation used in classical continuum mechanics. The packing fraction of C–S–H particles is very important as it is a determining factor.

Other papers in this issue are on additives. Additives improve the properties of concrete, such as rheology of fresh concrete, hydration rate, products, strength, durability, and so on. They also aid in reducing carbon dioxide emissions, a worldwide issue. Fine particles can control the particle size distribution and can get a closed packing structure, resulting in increased strength, low water/cement ratio and good flowability.

Additives come from a wide range of resources, such as by-products and local resources. These materials sometimes have strong individuality. The research on the use of these individual materials has been carried out individually, but the discussion should be done as general as possible.

The first two papers on this issue are on the control of particle size distribution and packing structure. Inozemtcev and

Korolev's (2016) paper is on the application of hollow microsphere particles for high-strength lightweight concrete. The use of microspheres was proposed to make a close-packed structure with low deformation. A grinded silica powder (ssa: 700–800 m²/kg), microsilica ($d < 10^{-6}$ m) and aluminosilicate hollow microspheres were used.

Long *et al.* (2016) report on the effects of the addition of nanoparticles of SiO₂, Al₂O₃, Fe₂O₃ and CaCO₃. On the mechanical strength, hydration and pore structure.

Chand *et al.* (2016) report on paraffin wax addition in concrete in order to mitigate the water evaporation to surroundings. It assists the self-curing of concrete. Very large molecule wax does not dissolve in water, so it does not affect the hydration.

The paper by Pyatina and Sugama (2016) concerns the application of fly ash in ordinary Portland cement (OPC) and the resulting resistance to thermal shock. It is for the materials of geothermal wells, which are sometimes exposed to temperatures of several hundred degrees. The hydration products of OPC and class-F fly ash activated with sodium metasilicate, soda ash and sodium sulfate were sodium calcium aluminium silicate, formed at a high temperature of 300°C. The crystallinity of these compounds was decreased with thermal shock.

The last topic concerns an analytical methodology, selective dissolution analysis. Separation and analysis of phases are very important to investigate the properties of materials. It is very difficult to separate phases completely, so selective dissolution methods are often used. It has to be put in our mind that this method uses the relative differences of solubility or rate of solution.

The last report in this issue is reported by Ma *et al.* (2016) on the separation of sulfate phases. Water can determine the content of alkali sulfate. A 50% ethanol solution can determine the content of easy soluble sulfates but prevents the dissolution of gypsum and the hydration of sulfate with calcium aluminate during extraction, and gypsum was analysed with saturated sodium carbonate solution.

Scientific knowledge is established on the study of natural phenomena and experimental results, so even established knowledge could be overthrown by a future discovery (e.g., the incorrect assumption that neutrinos did not have mass). Therefore, when a scientific theory is composed, there is always the possibility of being proved wrong. In the

mathematics field, a hypothesis will be certified from theorem and that will be understood as true, never to be overthrown; whereas, the scientific method is always advancing because knowledge and understanding is constantly corrected by new discoveries.

References

- Chand MSR, Kumar PR, Giri PSNR, Kumar GR and Rao MVK (2016) Influence of paraffin wax as a self-curing compound in self-compacting concretes. *Advances in Cement Research* **28(2)**: 110–120, <http://dx.doi.org/10.1680/jadcr.15.00062>.
- Inozemtcev AS and Korolev EV (2016) A method for the reduction of deformation of high-strength lightweight cement concrete. *Advances in Cement Research* **28(2)**: 92–98, <http://dx.doi.org/10.1680/jadcr.15.00049>.
- Jingjing Z, Qing Z, Dan H and Feng S (2016) A peridynamic approach for the simulation of calcium silicate hydrate nanoindentation. *Advances in Cement Research* **28(2)**: 84–91, <http://dx.doi.org/10.1680/jadcr.15.00018>.
- Long G, Shi Y, Ma K and Xie Y (2016) Reactive powder concrete reinforced by nanoparticles. *Advances in Cement Research* **28(2)**: 99–109, <http://dx.doi.org/10.1680/jadcr.15.00058>.
- Ma Y, Qian J, Yang S and Deng L (2016) Measuring the distribution of sulfate phases in cement. *Advances in Cement Research* **28(2)**: 132–140, <http://dx.doi.org/10.1680/jadcr.15.00031>.
- Pyatina T and Sugama T (2016) Resistance of fly ash–Portland cement blends to thermal shock. *Advances in Cement Research* **28(2)**: 121–131, <http://dx.doi.org/10.1680/adcr.15.00030>.
- Zhou J, Huang J and Jin L (2016), Nano–micro modelling of mechanical properties of cement paste based on molecular dynamics. *Advances in Cement Research* **28(2)**: 73–83, <http://dx.doi.org/10.1680/adcr.15.00048>.