In this issue

Cool and see

A continuing problem with ascribing a short non-bonded distance X--Y in molecular crystals to an attractive intermolecular contact is that it is usually impossible to make out, from just looking at a single crystal structure, whether the atoms X and Y want to come together in the crystal and form such an attractive contact, or whether they merely happen to come together, or whether they are even forced to come together because of other factors that operate within the crystal. In the latter case, the short contact X--Y would actually be repulsive. A part of the controversy surrounding weak C-H--O hydrogen bonds is that some short H--O distances arise from repulsive forced contacts. How does one make out the difference between a short C-H--O contact that is a true hydrogen bond and an equally short contact that results from a forced approach of a C-H group and an O-atom? The article by Thakur et al. (page 793) shows a way out of this dilemma. It is a property of all true hydrogen bonds that they become shorter and more linear as one cools the sample. This is because in real hydrogen bonds an electropositive H-atom screens the negative charges on two adjacent electronegative atoms. A lowering of temperature lowers the energy of the hydrogen bond, and this in turn means that it becomes shorter and hence more linear. The authors have selected a very old example from the crystallographic literature of two isostructural crystals, the 1:1 molecular complexes of barbital with urea and acetamide, in which an N-H--O contact in the first crystal (which is indisputably a genuine hydrogen bond) is replaced with a C-H--O contact in the second one.

Both these interactions show a similar behaviour upon cooling—they become shorter. The conclusion is that the C-H--O bond in the barbital-acetamide co-crystal is a real hydrogen bond.

Ion beam for synthesis and modification of nanostructures

Avasthi and Pivin report (page 780) the role of energetic ions of energies from a few keV to hundreds of MeV in nanostructuring with the examples of nanostructures obtained by ion irradiation experiments at IUAC, Delhi and CSNSM, Orsay. They range from the use of ion or atom beams of a few keV to generate periodic ripples on surface or grow nanocomposite thin films by sputtering to the formations of an isotropic structures under swift heavy ion (SHI) impacts. SHI has unique feature of creating ion track in insulators of dimension from a few nm to about 10 nm. SHI irradiation of polymers or fullerenes creates strings of carbon particles or wires useful as nanococontacts or field emission tips. The elongation of noble metal particles embedded in insulators attracts the attention for the design of light filters or waveguides. The SHI irradiation of silica film containing Fe nanoparticles, transform the magnetic easy axis from in-plane to out-of-plane, which is of interest for the perpendicular magnetic recording of information. The unique feature of SHI is used to engineer the size and shape of the metal nanoparticles embedded in silica matrix.

New technologies for strengthening damaged reinforced concrete structures

More and more the problem of strengthening damaged reinforced concrete structures becomes a priority. One of the well-known methods to accomplish this is structural consolidation by using gunning procedure.

By highlighting the shortcomings of this type of equipment, the most important one being the fact that the mixture does not have a continuous and homogeneous flow, Giusca and Corobceanu show (page 829) the possibility of making new devices that try to diminish this deficiency as much as possible.

In order to carry out the batching of the continuous cement-aggregate mixture flow, the device is composed of a dosing chamber which creates a separate area in which each amount, isolated through a cell, is continuously taken from there. To realize the best composition of the dry aggregate-cement components with water, a nozzle is provided at the end of the flow; the nozzle has an area where the water flows at a pressure which is higher than air from the discharge hose.

Following the tests performed in laboratories to measure the quantity of the aggregate-cement-water components, and the in situ studies to observe the quality of the flow of gunited mixture, the authors report an improved quality in relation to its homogeneity.