In this issue

Predicting transition pressures

The recent advances in the diamond anvil cell technique permit pressurization of solids up to a few hundred gigapascals. Large pressure gradients exist in the pressurized specimen and the peak pressure is localized over a small area, 5–10 μm in diameter. The use of intense X-ray beam from a synchrotron source makes it possible to obtain high resolution X-ray diffraction data from the peak-pressure region of the specimen. Such data have led to the identification of the crystal structures of the high pressure phases in solids. The observation of pressure-induced transitions has stimulated theoretical work. Attempts have been made to analyse the stability of the crystal structures under high pressure. The free energy of the structure at one atmosphere is calculated as a function of pressure, and the calculations are performed for a few plausible structures for the high pressure phase. The original structure is expected to transform to the structure with the lowest free energy. One uses several guidelines which are available in the literature for guessing the structure of the high pressure phase. The much improved formalism based on the density functional approach combined with high speed computational facilities is capable of providing reliable estimates of the energy difference between two structures, which is often small for the pressure-induced transitions. The calculated transition pressures for many systems agree well with the corresponding experimental values. For some systems the predicted transitions were observed subsequently. The article by Gupta *et al.* (**page 399**) reviews the work in this field, the emphasis being on the work done at BARC, Bombay. An agreement between the theoretically predicted and experimentally observed structures and transition pressures gives credence to the theoretical formalism. The cause of any disagreement must surely be traced to assumptions on which the theory is based. The agreement between the theory and the experiments establishes the theory, whereas in disagreement lies the scope for the further development of the theoretical formalism.

Estimating levels of pollution: expert vs expert, model vs model

Few controversies in the recent times have been more acrimonious than those between the pro-development and pro-environment protagonists. Announcement of any new major project invariably creates a storm, with the pro-development lobby welcoming it as a harbinger of prosperity, and the environmentalists condemning it as yet another agent of doom and destruction. The most tragic aspect of this situation is that one does find sincere and committed scholars on both the sides of the debate, each convinced of the soundness of his or her own stand, and of the hollowness of the opponents' stand. How, then, can rational decisions be made?

The first step is to express the perceived good or ill effects in some objective and quantitative manner. For example, instead of hysterical slogans ('highly polluting') and bland assurances ('almost totally non-polluting'), the debate should be about quantities such as the expected levels of concentrations of pollutants. This task should be (and often is) carried out by technical experts, who using the time-tested engineering principles, can estimate such parameters for assessing the extent of pollution by any specific installation.

There are, however, experts and experts, each with his or her battery of methods. Often, there is good agreement among results obtained by different experts, but not always. A particularly startling example is described by Padmanabhamurty and Chakrabarty (**page 419**). Using the available information on the thermal power plant at Dahanu (e.g., stack height, average wind speed, etc.), they have estimated two simple but crucial quantities; the distance from the power plant at which the concentration of a pollutant would be maximum, and the value of this maximum concentration. The eight different models explored by Padmanabhamurty and Chakrabarty predicted concentrations ranging from 8×10^{-19} to 0.70, a variation perhaps from highly salubrious to the absolutely lethal.

As judged by the holy touchstone–potential for making falsifiable predictions–the models are as scientific as anything can be, yet taken together, they apparently seem to have so little to offer towards making a rational real-life decision. To take a more positive view, when it comes to estimating pollution levels, Padmanabhamurty and Chakrabarty not only highlight the need to critically examine the existing models, but also show how such a scrutiny can be carried out, and, more importantly, what more needs to be done.