GUEST EDITORIAL

AND THE IMAGE WAS SIMULATED

It is now widely accepted that in order to determine how and with what degree of confidence a high resolution electron micrograph can be interpreted, it is necessary to perform a numerical image simulation. Unfortunately, this has its own problems. Multislice diffraction and imaging calculations can easily go wrong, particularly with the large cells required for what is perhaps the current cutting edge, namely simulation of surfaces or lattice defects to determine atomic coordinates. The two requirements of inclusion of high-angle scattering (to allow the diffraction calculation to converge) and large real space arrays (to prevent unphysical wraparound effects, primarily in the imaging) conflict. Unless very large arrays are used, it is impossible to meet both requirements. Simply to read in a paper that the image was simulated and then see a result is not enough. We need to know what approximations or assumptions were made.

How can we deal with this problem? If we were dealing with experimental rather than theoretical results the answer would be obvious. We would insist that the experimental technique was described. This allows other workers both to repeat the experiments and to gauge the merit of the work. It appears reasonable to insist that the same criteria should be applied to theoretical calculations. Two or three sentences giving cell size, sampling, slice thickness, imaging parameters and methods, what programs were used (since some contain dubious approximations) and any other details should be adequate.

Time for some standardization, either in editorial policy or in the refereeing?

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[Editor's note: We agree, and we hope that authors and referees will take heed.]