Comparison of convolutional and restoring algorithms for crystal structure determination in melt crystallisation modelling

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The method of molecular dynamics (MD) makes it possible to study the behaviour of various materials at the micro level. The processes occurring in a substance when subjected to intense flows of energy are difficult to analyse experimentally, whereas the MD method makes it possible to follow every atom, every incipient defect. But it is not enough to perform a numerical experiment, one must analyse calculation results, and this can only be done if one has efficient algorithms for handling data on billions of atoms in a simulated sample. One of such algorithms are algorithms for determining the crystal structure.

In this paper a comparison of convolutional and restoring algorithms for determining the crystal structure has been carried out. Both shock loading of the sample and heating to a temperature above the melting point have been simulated. In the considered examples the atoms belonging to BCC, HCC, HPC crystal lattice and icosahedral environment were determined.

The Adaptive Template Analysis method (ATA) [Sapozhnikov 2008] developed at RFNC-VNIITF, which is the first restoring method to determine the crystal structure, has surpassed both the most common convolution method—ACNA [Stukowski 2012], as well as the most common restoring method—PTM [Larsen 2016].