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Molecular Mechanics Simulations of Carbon Nanostructures Using Multi-Scale Boundary Conditions

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A new method of Multi-Scale Boundary Conditions (MSBCs) is applied to Molecular Mechanics simulations of carbon nanostructures such as graphite sheets and diamond. The method allows simulation of a deformable boundary, thus reducing the size of computational domain and, consequently, cost of computations. The approach is particularly effective in cases when deformation is localized in a relatively small region. The idea of the method is based on Fourier analysis of regular atomic structures and assumption of small (linear) deformations. However, this assumption has to hold in a small vicinity of the deformable boundary, where MSBCs are applied, whereas large deformations (including plasticity) are allowed inside the reduced domain and far enough from the deformable boundaries. The method is tested on model problems and the results are in good agreement with the full domain solutions. Currently, effort is being made to apply this method to simulate real-life experiments on nanoindentation of diamond and layered graphite.

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