Utilization of atomistic submodel in molecular dynamics stress analysis in single layer graphene

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Commonly used continuum models, implemented within finite elements method (FEM), are not suitable to predict the complex nature of stress distribution in atomistic systems around geometrical and structural discontinuities. To utilize the calculation speed and convenience of FEM, a framework that allows accurate description of the stress distribution in regions free of discontinuities, we have developed an atomistic submodel (AS). AS is placed in the global FEM model around the defects. This way calculation speed of FEM and accuracy of molecular dynamics, used to analyze stress within AS, are achieved.

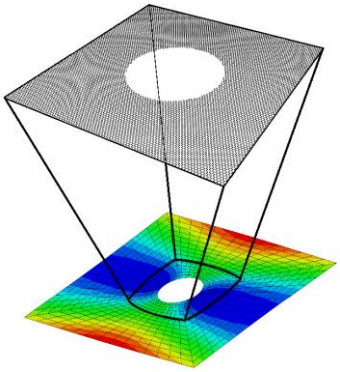

Figure 1, Placement of atomistic submodel within the finite element global model

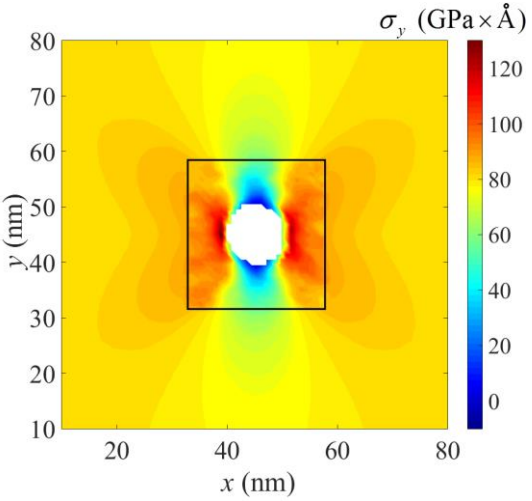

Figure 2, Stress distribution around the circular opening in single layer graphene, stress within the rectangle is derived from atomistic submodel and the rest from the finite element model