Abstract Submitted
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Toward Distinct Element Method Simulations of Carbon Nanotube Systems[1] EVGENIYA AKATYEVA, TYLER ANDERSON, ILIA NIKIFOROV, University of Minnesota, DAVID POTYONDY, Itasca Consulting Group, ROBERTO BALLARINI, TRAIAN DUMITRICA, University of Minnesota — We propose distinct element method modeling of carbon nanotube systems. The atomic-level description of an individual nanotube is coarse-grained into a chain of spherical elements that interact by parallel bonds located at their contacts. The spherical elements can lump multiple translational unit cells of the carbon nanotube and have both translational and rotational degrees of freedom. The discrete long ranged interaction between nanotubes is included in a van der Waals contact of nonmechanical nature that acts simultaneously with the parallel bonds. The created mesoscopic model is put into service by simulating a realistic carbon nanotube ring. The ring morphology arises from the energy balance stored in both parallel and van der Waals bonds.

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