

Abstract Submitted  
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**Accurate atomistic potentials and training sets for boron-nitride nanostructures** ISAAC TAMBLYN, National Research Council of Canada, University of Ontario Inst. of Tech — Boron nitride nanotubes exhibit exceptional structural, mechanical, and thermal properties. They are optically transparent and have high thermal stability, suggesting a wide range of opportunities for structural reinforcement of materials. Modeling can play an important role in determining the optimal approach to integrating nanotubes into a supporting matrix. Developing accurate, atomistic scale models of such nanoscale interfaces embedded within composites is challenging, however, due to the mismatch of length scales involved. Typical nanotube diameters range from 5-50 nm, with a length as large as a micron (i.e. a relevant length-scale for structural reinforcement). Unlike their carbon-based counterparts, well tested and transferable interatomic force fields are not common for BNNT. In light of this, we have developed an extensive training database of BN rich materials, under conditions relevant for BNNT synthesis and composites based on extensive first principles molecular dynamics simulations. Using this data, we have produced an artificial neural network potential capable of reproducing the accuracy of first principles data at significantly reduced computational cost, allowing for accurate simulation at the much larger length scales needed for composite design.

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