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**Simulations of amorphous nanoparticles: the effect of shape on surface structure and subsequent interactions with the surroundings** SUSAN FULLERTON, CHUNXIA CHEN, JANNA MARANAS, The Pennsylvania State University — Molecular dynamics simulation is employed to study the effect of varying nanoparticle shape on the structure of boron oxide nanoparticles, and their subsequent influence on surrounding polyethylene oxide. While previous studies have focused on crystalline nanoparticles, this study is unique because the nanoparticles are amorphous. Shape has been shown to affect the electrical and optical properties of nanoparticles, in addition to the structure and dynamics of polymers surrounding nanoparticles. In this study, two nano-shapes of boron oxide are compared: a 16 angstrom diameter sphere, and a 16 x 16 x 16 angstrom cube. The networks are described by a short-range structure consisting of BO<sub>3</sub> units, while the intermediate-range structure is described by six-membered planar boroxol rings. Both the fraction of boroxol rings and their locations differ between the two nano-shapes. All planar boroxol rings within the spherical simulation are located on the interior, while planar rings within the cubic simulation aggregate to the cube walls. Structural differences also appear at longer ranges, including the formation of “layers” aligned parallel to the walls of the cube. We also investigate how varying the nanoparticle shape influences the structure and dynamics of the surrounding polymer.

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