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Title: A Tersoff potential with modified cutoff for pure and hydrogenated amorphous carbon and the friction laws at the nanoscale

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A Tersoff potential with modified cutoff for pure and hydrogenated amorphous carbon and the friction laws at the nanoscale Z. D. Sha, P. S. Branicio, Q. X. Pei, V. Sorkin, and Y. W. Zhang Institute of High Performance Computing, 1 Fusionopolis Way, 16-16 Connexis 138632, Singapore Recently, amorphous carbon (a-C) has attracted intense attention due to its wide application such as overcoat, tips, and tools. To model and simulate the structures and properties of a-C, a reliable interatomic potential is required. In the present work, we evaluate the accuracy of four different interatomic potentials, that is, the reactive empirical bond order (REBO), standard Tersoff, Tersoff/ZBL, and Tersoff with extended cutoff interatomic potentials, against experimental and first-principle data. The simulation results show that Tersoff potential with extended cutoff is the most accurate one in reproducing the structure and mechanical properties of a-C. Remarkably, this potential is also able to reproduce the structure and mechanical properties of hydrogenated amorphous carbon (a-CH). The calculated sp3 fraction as a function of density, as well as the pair correlation functions, and Young?s modulus as a function of density for both a-C and a-CH show excellent agreement with experimental data. And based on the above a-C structure, we also investigated the friction laws at the nanoscale. The tip and substrate are amorphous carbon materials. An understanding of how friction force depends on applied load and contact area at these scales is essential for the design of miniaturized devices with optimal mechanical performance such as heat-assisted magnetic recording system. In our work, we first integrate the vdw potential into Tersoff potential. And then we focus on the question of the surfaces passivated with different hydrogen concentration effect on the friction force versus load curve.