Effects of Hydrogenation on Mechanical Properties of h-BN: A Reactive Force Field Study

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Abstract

In the present work, reactive force field (ReaxFF) based molecular dynamics simulations were used to study the effect full-hydrogenation on mechanical properties of boron nitride nanosheets (h-BN). Our results show that fully-hydrogenated boron nitride nanosheet (h-BN nanosheet) show slight decrease in mechanical properties but still retains its mechanical strength up to large extent. Due to its high strength hydrogenated h-BN nanosheets can find applications in fields such as hydrogen storage and space programs.

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