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Graphene melting by molecular dynamics simulations BRAD STEELE, ROMAIN PERRIOT, VASILY ZHAKHOVSKY, IVAN OLEYNIK, University of South Florida — Mechanisms of melting of graphene were studied by molecular dynamics (MD) using two different interatomic potentials: the Reactive Empirical Bond Order (REBO) and recently developed Screened Environment Dependent (SED) -REBO potentials. Melting was investigated in two-dimensional (2-D) and three-dimensional (3-D) coordinate space. It was shown that the loss of long-range order and melting proceeds through generation and in-plane aggregation of Stone-Wales (S-W) defects in REBO-graphene, followed by the formation of a complex 3D network of carbon chains. Although S-W defects are also formed in the SED-REBO-graphene, they do not cluster. Instead, the melting proceeds through the formation of dangling bonds and vacancies. The melting temperature of graphene using REBO was found to be 5,200 K, whereas for SED-REBO it is lower by ∼800K. The melting in 2-D occurs at higher temperatures compared to 3-D because of in-plane geometrical constraints.

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