Reaction Molecular Dynamics Simulation on the Compatibility of Epoxy Resin with Oxygen under Impact Load

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Abstract

The conventional polymer material has a compatibility problem with liquid oxygen (solid oxygen), and it is easy to cause combustion and explosion under the action of the external impact load. To study the compatibility of different epoxy resins with liquid oxygen (solid oxygen), reaction molecular dynamics (RMD) was used to simulate the change of the cross-linked epoxy resin system under the impact of solid oxygen, the resin system consists of bisphenol A epoxy resin (DGEBA), bisphenol F epoxy resin (DGEBF), tetrahydrophthalic acid diglycidyl ester (711 epoxy resin) with 4-4'diaminodiphenyl sulfone (DDM) curing agent respectively. The temperature change and mass loss of the polymer under oxygen impact were extracted as the judgment indicators for compatibility. And the simulation results show that the stability order of the three epoxy resins is DGEBA>DGEBF>711 at the same crosslink density, which is in good agreement with the previous experimental results. The above results validate the feasibility of using reaction molecular dynamics to study the compatibility of polymer materials with oxygen and provide a new idea for the selection and modification of subsequent polymer materials.

Keywords： Reaction molecular dynamics Reax FF Epoxy resin Oxygen Compatibility