Formation of sp^3 carbon materials via thermal decomposition of PHC

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Poly(hydriodocarbyne), abbreviated as PHC, is composed of tetrahedrally hybridized carbon-based random network backbone, which follows the chemical formula of $(CH)_n$. In virtue of its high C:H ratio, PHC is a unique sp^3 carbon precursor, which facilitates pyrolysis to carbon materials with high contents of sp^3 hybridized carbon (i.e. diamond and diamond-like carbon). In this study, we aim to suggest plausible reaction mechanism and optimized synthesis-conditions by investigating the thermal decomposition of PHC at atomistic level using classical and reactive molecular dynamics simulations. Model systems of PHC thin film with different thickness were generated in a way to minimize strain. After that, pyrolysis of each model system was investigated in the temperature range up to 4000K. A step-by-step thermal decomposition process including bond association, bond dissociation and hydrogen gas generation were observed and time-dependent amount of each product was analyzed.