

Large-Scale Simulation on Ethylene Polymerization by Metallocene Catalyst System

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【Introduction】 Polyolefins represented by polyethylene (PE) and polypropylene (PP) are indispensable materials with certain social impact in countless beneficial ways. Metallocene based catalyst technology is expected to revolutionize the immense polyolefin industry, particularly in polyethylene and polypropylene markets. Metallocenes offer some significant process advantages and produce polymers with very favourable properties. Traditional classical molecular dynamics (MD) method cannot challenge the ethylene/ α -olefin polymerization process of metallocene catalyst system. In the present investigation, our new method successfully performed MD simulation on ethylene/1-butene polymerization over Ti metallocene catalyst system.

【Method】 MD simulation were carried out with the New-Ryudo program, which is an integrated classical MD software developed in our laboratory. The calculations were performed for 800000 steps with a time step of 0.5 fs, 473K and pressure was set to 50 MPa during the simulation (same with experimental conditions).

【Results and Discussion】 Under the experimental temperature and pressure, our New-Ryudo program successfully performed the ethylene/1-butene polymerization process by Ti metallocene catalyst. A complex model of one Ti metallocene[CpSi(CH₃)₂N(CH₃)TiCl₂], one methylaluminoxane (MAO), 300 ethylene molecules and 300 1-butene molecules was prepared as shown in Fig. 1. From our results, we observed that Ti metallocene react to MAO, then Ti active center[CpSi(CH₃)₂N(CH₃)TiCH₃] formed. After the Ti active center formation, ethylene/1-butene close to active center and ethylene/1-butene inserted to Ti active center (polymer chain growing as shown in Fig. 2). Our simulation results are in good agreement with the metallocene reaction mechanism obtained by experiment.

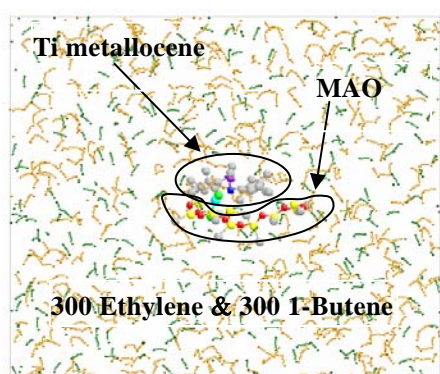


Fig. 1 Complex initial structure

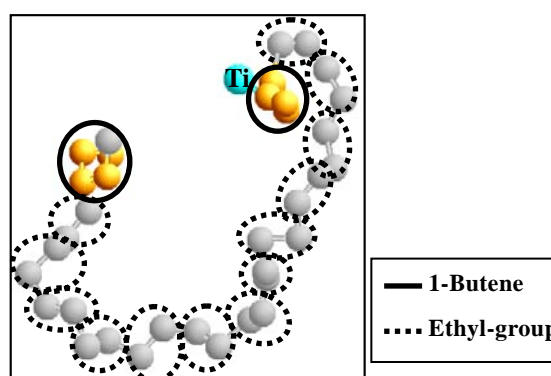


Fig. 2 Polymer chain growing (400ps)