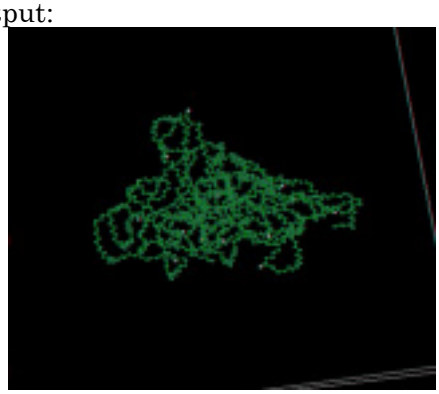
No. EAR3-022-01 First registration:2001/11/15 New:2001/11/15

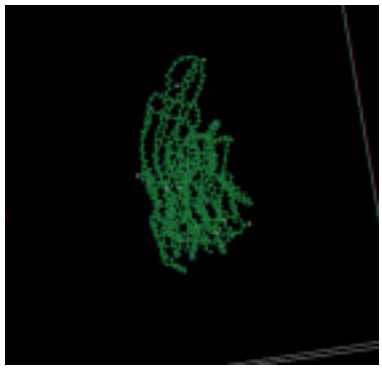
Title	The influence of short chain branching on polymer crystallization process -molecular dynamics simulation-
Researchers	Tatusya Shoji, Jun-ichi Takimoto, and Masao Doi
Purpose of this study	To investigate the influence of arrangement of and number of short chain branching on main chain on polyethylene crystallization process by using molecular dynamics simulation.
System (Material)	one chain of polyethylene ($C_{1000}H_{2002}$) replaced by the united atom model **sample name** / **architecture** / **branching arrangement** lin — linear (no branching) b10re — 10 methyl branching — regular b15re — 15 methyl branching — regular b15ra — 15 methyl branching — random
Program (including analysis)	COGNAC version 3 analysis: trajectory analyzer (order parameter、conformation)
Method & Some important input parameters	(Method) Coarse-grained molecular dynamics using united atom models potentials (Inputs) -polymer architecture(degree of polymerization) -united atom models potentials(bond ,bending, torsion, non-bond) -calculation conditions(temperature, density, time steps, etc...)
Advance & Problem	(Advance) We investigated the influence of arrangement of and number of short chain branching on main chain on the nucleation and growth process of crystallization of isolated one chain polyethylene by using molecular dynamics simulation. All of branched beads were swept out from inner lamella and finally located at the folding points of crystalline lamella interface. The arrangement and number of branching changed the averaged thickness of the lamella stem. We consider that it is possible to control the thickness of lamella by the primary structure of polymer.
References	[Manuscript] Submitted/Accepted(/) [Presentation at conferences (Meetings)] Polymer Preprints Japan (**49**(8), 2032 (2000)
KeyWords (in English)	molecular dynamics(MD) simulation , the united atom model , methyl branching , crystallization , the nucleation and growth interval of insertion,

Results (Remarks)

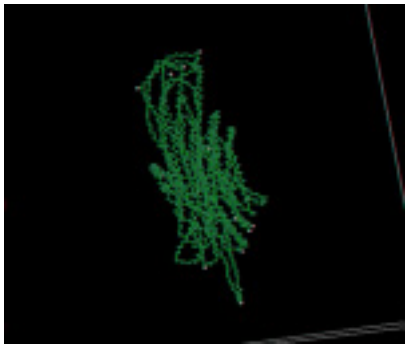
Output:



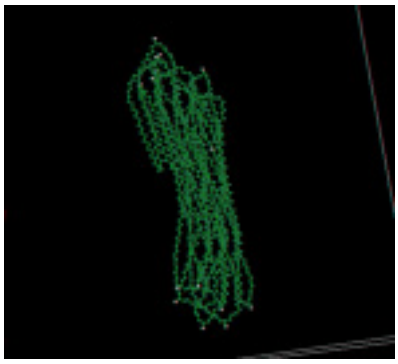
(a) t=0



(b) t=50ps



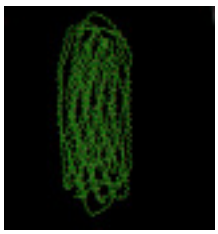
(c) t=100ps



(d) t=1ns

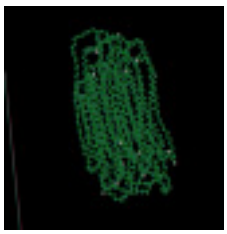
Fig.1 Snapshots of b15re until 1ns after quenching.

Fig.1 shows snapshots of b15re until 1ns after quenching. The crystallization process of the branched polymer consists two steps. In the first step, the branched parts are quickly pushed out from the random coordinates to surface of a coil, and give rise to fold as starting point of chain-folding, and form the local ordered stems. In the second step, the linear chain parts form gradually orderd structures and finally becomes crystalline lamella structures with chain-folded interfaces.

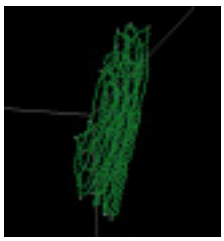


(a) lin

(b) b10re



(c)b15ra



(d)b15re

Fig.2 Snapshots of four sample after crystalization.

Fig.2 shows the final structures of the four samples after crystallization. The thickness of each sample was (a) 52, (b) 49, (c) 47, or (d) 71 Angstrom. Therefore we consider that it is possible to control the thickness of lamella by the primary structure of polymer.