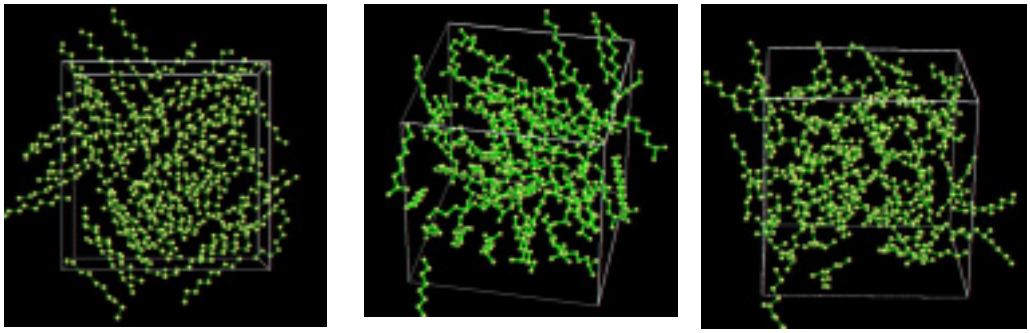
No. EAR1-006-01 First registration:2000/ 9/12 New: 2001/ 11/16

Title	Molecular dynamics simulation of alkane crystallization processes: - Effect of short-chain branching-
Researchers	T. Shoji, T. Aoyagi, H. Fukunaga, F. Sawa, J. Takimoto and M. Doi
Purpose of this study	The purpose of this study is to make clear the effects of short-chain branching in primary nucleation and growth processes of polymer by using molecular dynamics(MD) simulation method.
System (Material)	linear alkane: n-decane short-branched alkane 1: 2methyl-nonane short-branched alkane 2: 5methyl-nonane
Program (including analysis)	Program: COGNAC v1.3 Analysis: trajectory analyzer (order parameter, conformation analysis)
Method & Some important input parameters	(Method) Molecular dynamics simulation modeled by united atom model with empirical potentials. (Inputs) polymer architecture(degree of polymerization) united atom models potentials(bond ,bending, torsion, non-bond) calculation conditions(temperature, pressure, density, time steps)
Advance & Problem	(Advance) Ordered crystal structure was not observed for the branched chains by quenching to the temperature where the linear chain formed crystal. The suppression of the crystallization due to the branching was enhanced when the branching was located close to the middle of the backbone. (Problem) Observation of crystallization process for linear / branched chain's blend system could give useful information on the effect of the branching structure.
References	[Manuscript] Submitted/Accepted(/) Polymer Preprints Japan, Vol.48, No.14, 3955 (1999) 219th ACS National Meeting(2000) International Symposium on Platform for Designing High Functional Materials(2000)
KeyWords (in English)	molecular dynamics(MD) simulation , the united atom model , short-chain branching , crystallization , the nucleation and growth n-decane, 2methyl-nonane, 5methyl-nonane

Results (Remarks)

Output:



(a)n-decane (b)2methyl-nonane (c)5methyl-nonane

Fig.1 The snapshots of the different chains systems at 11 nano seconds after quenching to 180K from 420K. The n-decane chains (a) show ordered structure and create several of crystal domains. On the other hand, 2methyl-nonane chains (b) made the partial ordered conformations, but most of chains are still random.5methyl-nonane chains (c) have no ordering structures.

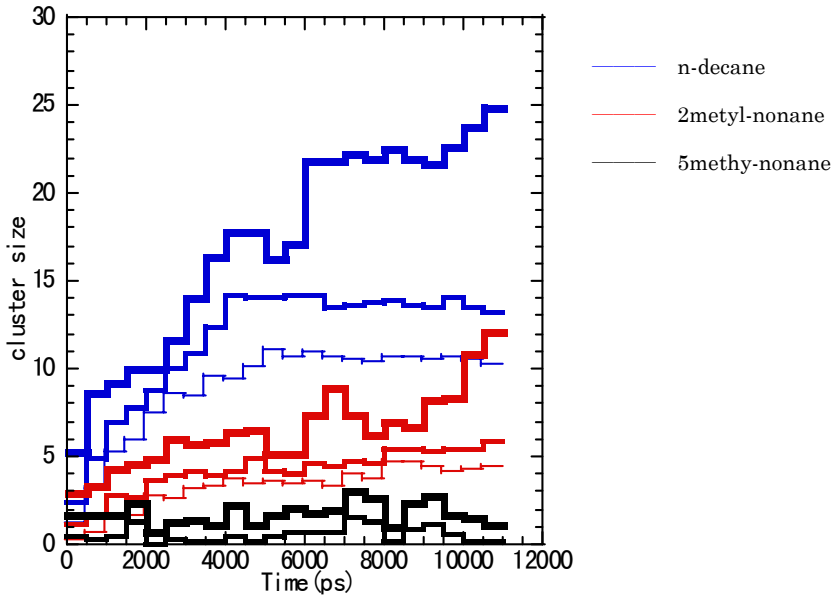


Fig.2 The crystal domain cluster sizes averaged each 500ps vs time. Thick lines represent maximum crystal domain cluster sizes, the middle thick lines the second largest, and the thin lines the third largest. The clusters of n-decane were created at once and grow stably with time until saturating. The clusters of 2methyl-nonane were created but the growth rates were slower. In the case of 5methyl-nonane, The cluster was hardly created. It is obvious that the positions of short-chain branching have influence and strongly hinder nucleation and growth in primary crystallization processes. The effect is prominent when the branching was located around the middle of the backbone.