Molecular Dynamics Study of Thermal Rupture of Linear Alternate Copolymer

김기웅, A. Ghosh, 이광순, 이원보*
서강대학교
(wblee92@sogang.ac.kr*)

We investigate the thermal rupture behavior of a linear alternating copolymer fixed at one end and pulled by a constant force at the other end by means of extensive MD simulation. The dependences of the first breakage time distribution and average rate of chain scission on the friction and the mass ratio of the constituent beads have been elucidated. The role of friction on healing/recombination has also been studied. The Arrhenian nature of the scission process has been confirmed and an estimate of the effective energy barrier has been made.