

**Название публикации:**

Theoretical investigation of polyethylene and butadiene rubber chain rupture process

**Авторы:**

Krisyuk, B.E.a, Mamin, E.A.b,c, Zyкова, A.K.b,c, Mastalygina, E.E.b,c, Popov, A.A.b,c

- a) Institute of Problems of Chemical Physics RAS, Chernogolovka, Moscow Region, 142432, Russian Federation
- b) Plekhanov Russian University of Economics, Moscow, 117997, Russian Federation
- c) Emanuel Institute of Biochemical Physics RAS, Moscow, 119334, Russian Federation

**Наименование журнала:**

AIP Conference Proceedings

Volume 2051, 12 December 2018, Номер статьи 020149

International Symposium on Hierarchical Materials: Development and Applications for New Technologies and Reliable Structures 2018; Tomsk; Russian Federation; 1 October 2018 до 5 October 2018; Код 143206

**Аннотация:**

The main attention of the article is focused on the chain-scission reaction of polyethylene and butadiene rubber in presence of chain deformation, especially when covalent bonds are strained. The enlargement of the bond or a fragment of chain has a significant influence on the rate of this process. The structure of the polymer also has an effect on the rate of the reaction. The quantum chemistry methods were used in order to consider the process and estimate bond rigidity and energy of bond rupture under different tension and deformation. These parameters were required to determine in what extent the reaction rate changed when tension was applied. © 2018 Author(s).

**Ключевые слова:**

-