Gradient Pattern Analysis of Simulated Short Chain Molecules

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ABSTRACT

Algebric and geometric methods from Gradient Pattern Analysis (GPA) theory [2-4] were applied for the first time for simulated molecular chains (using Fujiwara-Sato model [1]) with the objective of characterizing small symmetry breaking and phase disorder imposed due to thermal fluctuations. These fluctuations make it difficult to investigate the motion of the chains molecules under potential interaction (e.g. Lennard Jones potential).The effect of thermal fluctuations is simulated by means of the temperature of the heat bath in which chain molecules immersed (this parameter can be ranging from 0 to 400 K).

The objective of this paper is to introduce the Asymmetric Rigidity (R_A) as a new parameter for characterization of spatio-temporal relaxation of complex molecular systems. The parameter R_A is a function of both bath temperature and amount of asymmetries in the molecular gradient field. The sensitivity of the Asymmetric Rigidity is discussed taking into consideration possible mechanical effects due to an additional gravitational field.

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