A Simple “Sticky Disc” Model for Crystalline and Amorphous Networks

ADRIAN HUERTA, Arizona State University, NIKITA CHUBYNSKY, Universite de Montreal, GERARDO NAUMIS, Universidad Nacional Autonoma de Mexico, MICHAEL THORPE, Arizona State University — Using Monte Carlo simulations, we study the structural and thermodynamic behavior of a simple one component network forming model made up of “sticky discs.” Central and bond bending forces were included, modeling such interactions as a simple square well radial and angular three body term in the potential respectively. The main feature of this model is the ability to form crystalline and amorphous networks upon cooling, similar to that obtained using the so called WWW methodology to describe the network of some vitreous structures [1]. With the “pebble game” algorithm [2], we evaluate the number of degrees of freedom and the amount of stress in both the amorphous and crystalline structures. We discuss the connection between the configurational entropy (associated with the topology) and the degrees of freedom. Other effects such as elasticity of these structures are also discussed.