## DNA Cracks at the Region of Protein Binding Under the Action of Stretch

Qingjia Chi<sup>\*</sup> and Xinge Geng

Hubei Key Laboratory of Theory and Application of Advanced Materials Mechanics, Department of Mechanics and Engineering Structure, Wuhan University of Technology, China. \*Correspondence Author: Qingjia Chi. Email: qingjia@whut.edu.cn.

> The binding of DNA to protein in the cellular nucleus is a common phenomenon. DNA molecules will soften at the binding region when they adhere to proteins. Softening will affect the mechanical properties significantly. However, the mechanism underlying the mechanical softening remains to be explored. To understand the changes in the mechanical properties of DNA, the peridynamics technique can effectively capture the stress of the softened DNA under tensile forces. And later the results were verified by finite element computations. Utilizing the computations of perydynamics to reveal the stretch of the double-stranded DNA. The results demonstrated DNA was easy to be broken at the softening position. A continuous model of DNA double helix was established in the finite element solver ABAQUS. Under the action of the uniform tension, the strain at the DNA softening region was much larger than the strain at the un-softening region. And when the tensile strain amount reaches a certain level, the DNA chain would be cracked at the softening position. This also means that DNA cracks often occur in the softening region. The results showed that the mechanical strength of DNA was significantly reduced at the softening region, resulting in a large strain of DNA at the region. Moreover, the softening region was more prone to cracks and even breakage.

Keywords: DNA softening; peridynamics; finite element; crack