Peridynamic Modelling of Ruptures in Lipid Membranes

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ABSTRACT

Mechanical stress can cause biomembranes to form pores[1] or ruptures[2]. Under normal physiologic conditions, up to 25% of mammalian cardiac and skeletal muscle cells, and 6% of skin cells are in a damaged state, due to stretching and shearing[3]. Irreversible rupturing of cells has been associated with devastating diseases, e.g. muscular dystrophy[4]. We have shown in 2010 for the first time that a phospholipid double bilayer membrane on a solid support, in which the two individual bilayers are separated by a nanoscopically thin water layer, can form both floral and fractal ruptures[5]. The differences between the two established rupture modes in double bilayers have been related to the thickness of the water layer, as well as the quantity of interconnecting (pinning) sites between the two membranes of the double bilayer[5]. However, the extremely small fluid volume entrapped between the bilayers, which is on the order of femtoliters,[6] poses limits on experimental investigation. Further understanding of the two rupture mechanisms requires innovative approaches, models and experimental designs.

The lipid bilayer membranes involved are a few nanometers thick and can extend up to hundreds of micrometers laterally. With respect to their fundamental material properties, they can be considered to be two dimensional (2D) elastic sheets[7], with a large bending, and comparatively small stretching modulus. In an attempt to model, and consequently understand, the rupture dynamics of such membranes, we have applied a peridynamics approach with the aim of gaining deeper insights into the conditions and structural requirements for fracture formation in biological membranes. In particular, we apply a 2D membrane approximation of the three-dimensional state-based theory of peridynamics. This model has been implemented in a GPU parallelized mesh-free explicit code using the CUDA parallel computing platform. We highlight aspects of constitutive model development and demonstrate the model through numerical simulation.

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