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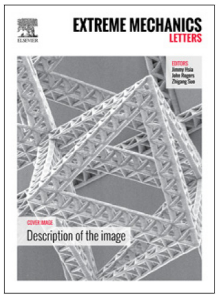

Packing of flexible nanofibers in vesicles

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Packing of flexible nanofibers in vesicles

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Abstract

Cellular packaging of flexible nanofibers, including natural cytoskeletal microtubules, actin filaments, synthetic nanotubes and nanowires, is of fundamental interest to the understanding of a wide range of cell activities, including cell shape control, cell movement, cell division, and nano-cytotoxicity. Here, we perform molecular dynamics simulations and theoretical analysis to elucidate how the geometrical and mechanical properties of a flexible nanofiber influence its encapsulation within a lipid vesicle. Our analysis indicates that the packing morphology depends on the length and stiffness of the nanofiber, the initial configuration of the nanofiber-vesicle system and the pressure difference across the vesicle membrane. We establish a packing phase diagram based on three distinct vesicle morphologies in equilibrium, including a non-axisymmetric dumpling-shaped vesicle with a strongly curved nanofiber, a cherry-shaped vesicle with a tubular membrane protrusion enclosing a significant portion of the nanofiber, and an axisymmetric lemon-shaped vesicle with a pair of protruding tips induced by the encapsulated nanofiber.

Keywords: nanofiber packing; nanofiber-vesicle interaction; membrane protrusion; nanofiber buckling; cell shape; molecular dynamics simulations

1. Introduction

Packing of flexible fibrous nanomaterials in a soft confinement such as vesicles and vesicular compartments is ubiquitous in biology and plays fundamental roles in many cellular functions. For example, the packing of cytoskeletal microtubules and actin filaments provides mechanical support and driving forces for cell movement, regulates cell shape and facilitates chromosome segregation in cell division [1-6]. Packing of synthetic one-dimensional nanomaterials like carbon nanotubes in cells or subcellular organelles is found to be crucial to their cytotoxicity [7, 8].

Experimental studies such as morphological transformation or evolution of liposomes [5, 6, 9, 10] and active nematic vesicles [11] induced by microtubules have demonstrated that the bending stiffness [5, 11, 12] and length [9-11, 13, 14] of an encapsulated nanofiber are two essential properties that regulate its packing within a vesicle. Representative morphologies of

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