Analysis of Carbon Nanotubes and Graphene Nanoribbons with Folded Racket Shapes

ANDY BORUM, Engineering Science and Mechanics, Virginia Tech, RAYMOND PLAUT, Civil and Environmental Engineering, Virginia Tech, DAVID DILLARD, Engineering Science and Mechanics, Virginia Tech — When carbon nanotubes and graphene nanoribbons become long, they may self-fold and form tennis racket-like shapes. This phenomenon is analyzed in two ways by treating a nanotube or nanoribbon as an elastica. First, an approach from adhesion science is used, in which the two sides of the racket handle are assumed to be straight and bonded together with constant or no separation. New analytical results are obtained involving the shape, bending energy, and adhesion energy of the self-folded structures. These relations show that the dimensions of the racket loop are proportional to the square root of the flexural rigidity. The second analysis uses the Lennard-Jones potential to model the van der Waals forces between the two sides of the racket. A nanoribbon is considered, and the interatomic forces are integrated along the length and across the width of the nanoribbon. The resulting integro-differential equations are solved using the finite difference method. The racket handle is found to be in compression and the separation between the two sides of the racket handle decreases in the direction of the racket loop. The results for the Lennard-Jones model approximately satisfy the relationship between the dimensions and the flexural rigidity found using the adhesion model.

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