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MODELLING JOINING OF VARIOUS CARBON NANOSTRUCTURES USING CALCULUS OF VARIATIONS

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Abstract. Numerous types of carbon nanostructure have been found experimentally, including nanotubes, fullerenes, nanocones and graphene. These structures have received much attention for their potential application in various nanoscale devices. The joining of different types of nanostructures may lead to further new structures with even more remarkable properties with possibly more potential applications. Using the calculus of variations, this paper models the join between different types of carbon nanostructures, namely carbon nanocone and fullerene, two nanocones, graphene and nanocone, fullerene and graphene, and nanocone and two parallel sheets of graphene. A perfect join configuration of absolute minimum energy is found in some circumstances. In general, the joining of these structures can be categorised into one of two models which are based on the curvature of the join profile. We refer to Model I when the join profile only involves positive curvature and Model II for the case of both positive and negative curvatures. We consider three cases of joining nanocones with a spherical cap: exactly half, more than half and less than half of a sphere. For two nanocones, we investigate the join between two symmetric carbon nanocones and the join between two nanocones which have different cone angles. These composite structures may be useful for the design of probes for scanning tunnelling microscopy and other nanoscale devices, such as carriers for drug delivery, and pores for gas and liquid separation.

1 Introduction

Nanostructured materials are of interests to many research fields due to their physical, chemical and electronic properties [1, 2]. In particular, carbon