Energy analysis of nanocarbon materials with defect structure using NEB method

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Abstract

Graphene sheets (GSs) with excellent mechanical and electrical properties are used in a wide range of applications such as electronic devices, solar cells and so on. Recently, lattice defects (5-7 defects) have been discovered in GS, which affect the strength of GS. The aim of this study is to find the minimum energy pathway using the NEB (Nudged Elastic Band) method to investigate the energy required for GS to change its structure. The NEB method is used to find the minimum energy path of the transition state. Two analytical models were created in this study: a schematic diagram of the first model is shown in Figure 1. In Figure 1, I. is the length of the model which is $L_x = L_y = 200$Å. II. is the number of six-membered rings between the upper and lower dislocations which is 0, 1, 2, 3, and 4 six-membered rings. III. is the distance between dislocation pairs which is 8 six-membered rings. IV. is the number of dislocation pairs is four kinds: 1, 2, 3, and 4. Based on the molecular dynamics method, we used NEB method to calculate the potential energy of GS with dislocation pairs of 1, 2, 3, 4, during the process of dislocation pairs in GS separating from each from 0 to 1, 1 to 2, 2 to 3, and 3 to 4 six-membered rings (II. in Fig.1). The results of the energy analysis for the entire transition state are shown in Figure 2. The overall energy of the transition state increases as the number of dislocation pairs increases. The overall energy of the transition state changes little when the angle between the dislocation pairs is changed. The formation energy and activation energy both increase as the number of dislocation pairs increases.

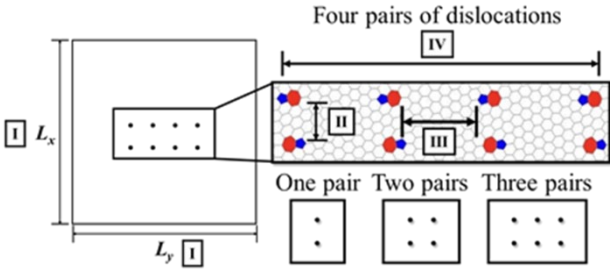

Fig.1 A schematic diagram of the first model

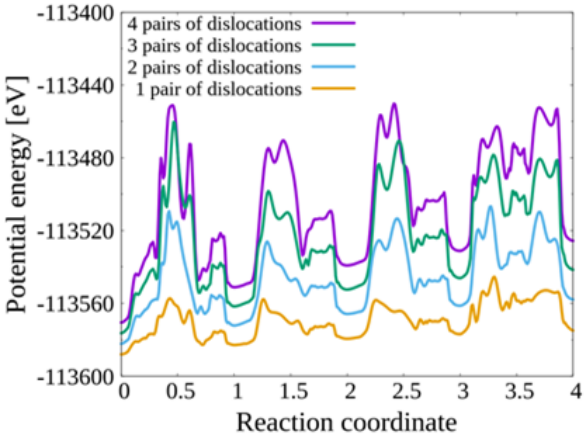

Fig.2 The results of the energy analysis

Keywords: GS, NEB, Formation energy, Activation energy