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Application of atomic simulation methods on the study of graphene nanostructure fabrication by particle beam irradiation: A review

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ABSTRACT

Graphene has been demonstrated to have enormous potential applications. The realization of the applications is closely related to the fabrication of graphene nanostructures. In this paper, the recent studies of graphene nanostructure fabrication by particle beam (laser beam, electron beam and ion beam) irradiation have been reviewed, for which the usage of atomic simulation methods is focused on. Firstly, the interaction mechanism between particle beam and graphene is discussed. Then based on the different interaction mechanisms, the atomic simulation models were built to figure out the feasibility of using particle beam irradiation to dope graphene, join graphene and fabricate graphene nanopore. The limitations of the present models are analyzed at last, and the possible future research directions are forecasted. This review aims at stimulating further research on this subject.

1. Introduction

Graphene is a single carbon layer in which the sp^2-bonded carbon atoms tightly pack into a honeycomb crystal lattice. As a two-dimensional new material, graphene has been demonstrated to have outstanding optical [1–3], electrical [4–6], thermal [7–9] and mechanical properties [10–14]. These extraordinary properties enable graphene to be a special candidate for the applications in different areas, such as solar cells [15–17], transistors [18,19], transparent electrode [20–23], biosensors [24–26] and so on. Fig. 1 depicts some of the potential applications for graphene in various fields [27]. From Fig. 1, it can be seen that most of the applications require the fabrication of graphene nanostructures. For example, to construct a graphene based field effect transistor with adjustable properties, we need to precisely cut the graphene piece into specific width [15]. And also the application of graphene in the DNA sequencing needs to fabricate a nanopore structure in the graphene sheet. The graphene nanopore structure could make it feasible to conduct gene sequencing at a single-base resolution, which is unreachable for other nanopore technologies [28]. Some of the applications, like automobile, aerospace require large size graphene with controllable shape. Graphene joining could efficiently control the shape and size of the graphene structure [29,30]. Meanwhile, the doping of graphene can manipulate the electrical and optical properties of graphene [31], which could enable the application of graphene in quantum devices, solar cells. It is no exaggeration to say that the applications of graphene cannot be realized without controllable processing of graphene nanostructures.

For the graphene nanostructure fabrication, a number of physical and chemical methods have been proposed. Such as the joining of graphene under current joule heat [32], fabrication of graphene nanopore by block copolymer lithography [33], and doping of graphene using chemical vapor deposition method [34]. The existing methods have shortages to some degree, which include the complex operation and high demand for equipment (graphene joining), limited processing accuracy and easy to bring contamination (graphene nanopore fabrication), incapable of doping a specified region (graphene doping), and so on. Particle beam (in this paper, particle beam refers to laser beam, electron beam and ion beam) processing technology has the characteristics of high precision, high efficiency, mature control method, and fast developing speed. The application of particle beam irradiation on the processing of graphene nanostructures could present obvious advantages. For instance, for the graphene joining, particle beam species can be controlled to achieve the different forms of joint, and the performance of joint can also be adjusted by changing the particle beam parameters. For the doping, low-energy ion implantation can be used to dope graphene at the specified location with designated concentration.

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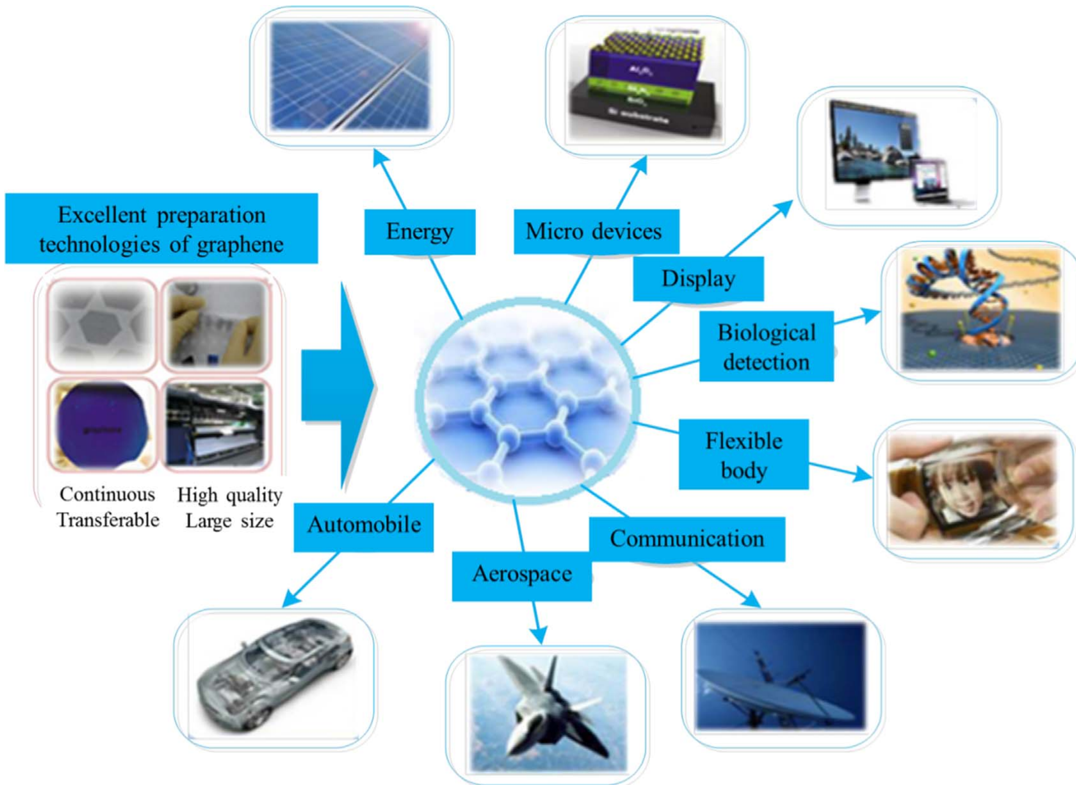

Fig. 1. Applications of graphene in different fields [27].

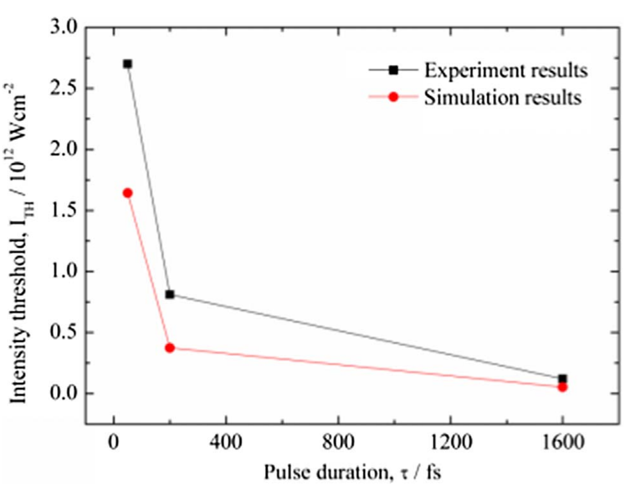

Fig. 2. Intensity thresholds for single-shot laser damage of graphene from MD simulation [51], and experiment [52].

Meanwhile, focused electron beam and ion beam can be used to get high precision nanopore structure.

There are some experimental studies conducted to investigate the mechanism and phenomena of graphene nanostructure fabrication by particle beam irradiation. In 2013, Ye [29] reported the using of laser beam irradiation to connect two graphene flakes, which is the first experimental study related to the graphene joining by particle beam irradiation. In 2017, we figured out the possibility of graphene joining by N ion beam irradiation, and uncovered a different joining mechanism from laser irradiation method [35]. It was demonstrated that graphene can be doped by laser [36], electron beam [37] and ion beam irradiation [38–40]. Especially for ion beam, N, B, F, P elements were successfully doped into graphene to induce the donor or acceptor doping. Besides, the focused electron beam shows its capability to process nanoscale pore in graphene from experimental investigations [41,42]. As a nanomaterial, most of the phenomena during the interaction between graphene and particle beam irradiation happen at nano or even sub-nano scale, and in a very short time, which couldn't be thoroughly captured by the present experiment technologies. Atomic simulation methods, like molecular dynamics (MD) simulation, first principle (FP) calculation, and Monte Carlo (MC) method have led to great strides in the description of nanomaterials. By using these atomic simulation methods, the microscopic phenomena and mechanisms of graphene processing under particle beam irradiation could be uncovered by using small atomic system.

This review focuses on the atomic simulation study of graphene nanostructure processing by using particle beam irradiation method. Three aspects of graphene nanofabrication are covered: graphene doping, graphene joining and graphene nanopore fabrication. The readers should notice that there are already several review articles on this theme focusing on the irradiation-induced effects in carbon nanosystems [43–45], atomic simulations of irradiation effects [46], and atomic scale structural defects in graphene [47,48]. On one hand, this review can have a complementary role to these published papers due to the rapid development and newly emerged discoveries in this field. On the other hand, this review focuses more on the modelling side, especially on uncovering the underlying mechanisms for fabrication of graphene nanostructures, which have significant importance for graphene applications, while rarely talked before. Through this review, we try to analyze the most recent research progress, and stimulate further future research on this subject.

2. Interaction mechanisms between particle beam and graphene

The irradiation of laser beam onto graphene could induce the resonance energy transfer from the laser photon to the electrons in graphene, then the transfer of energy between electrons and phonons in graphene lattice. This energy transfer process happens in a very short time (femtosecond time scale). The kinetic energy of carbon atoms will