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Molecular dynamics simulations of ion-irradiation induced deflection of 2D graphene films

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Abstract

Ion-irradiation induced surface stress generation and the resulting deflection of 2D cantilever graphene films is studied using molecular dynamics (MD) simulations. The simulation results show that the free-end deflection is strongly dependent on the kinetic energy of the incident ions. At low incident energies ($\ll$10 eV), the graphene film bends towards the irradiated side (upward deflection in our simulations); a transition from bending towards the irradiated side (upward deflection) to bending away from the irradiated side (downward deflection) occurs when the incident energy is $\sim$10 eV; the downward deflection peaks at $\sim$50 eV. Further increases of the incident energy cause the magnitude of downward deflection to decrease. The evolution of free-end deflection with respect to the number of incidences is also dependent on the incident energy. The dependence of the deflection behavior of the graphene films on the incident energy revealed by our atomistic simulations suggests the generation of intrinsic stress of different levels in the growing films. Such behavior may be attributed to competing mechanisms of production and annihilation of interstitial- and vacancy-like defects in the growing film. Understanding the dependence of thin film deflection on the incident energy provides guidelines for controlling thin film shapes at the nanometer scale using ion-beam machining.
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Keywords: Molecular dynamics simulations; Ion-beam machining; Deflection; Interstitials; Vacancies

1. Introduction

In applications of micro-opto-mechanical systems (MOMS) and nano-electro-mechanical systems (NEMS), it is often desirable to tailor the contour shape of free-standing thin films on the nano-meter scale so as to minimize surface adhesion and friction between two mating surfaces with nanometer gaps, or to ensure uniformly directed light reflection. However, residual strains are often introduced into these thin films during

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their manufacturing processes, resulting in a radius of curvature on the order of micrometers, which becomes one of the major concerns in aforementioned applications. It has recently been demonstrated (Bifano et al., 2002) that ion-beam machining can effectively incorporate a high-level residual stress to the thin films by modifying their subsurface nanostructures, thereby presenting a unique technique for nanoscale control of the contour shape of free-standing thin films. Therefore, it is both fundamentally and practically critical to uncover the underlying mechanisms responsible for curvature formation and elimination in free-standing thin films during ion irradiations. During ion bombardment, if the impacting ions do not penetrate into the substrate, the process is referred to as thin film deposition or thin film growth; whereas if the impact ions penetrate significantly into the substrate, the process is called ion irradiation. Irradiation could occur under other conditions such as in nuclear reactor structures where high energy particles (mostly neutrons but sometimes ions, too) penetrate deep into the surface of the reactor structure.

Various experimental techniques have been used to monitor stress evolution during ion bombardments (Bifano et al., 2002; Volkert, 1991; Zhu et al., 2003). Such experiments typically involve *in situ* measurement of film curvature, with which the stress in the thin film can be determined using the Stoney's equation. It was generally observed in these experiments that ion bombardment amorphizes the film surface and the steady-state stress of the films is strongly dependent on the kinetic energy of the incident ions. Volkert (1991) observed that in a silicon film upon MeV ion irradiations the compressive stress increases and peaks as the amorphous regions are formed. The compressive stress then decreases and reaches a steady-state value as amorphization continues and eventually saturates. Lee et al. (1999) observed that ion irradiations result in a decrease in the compressive stress in diamond-like carbon films, and the steady-state stress is slightly tensile. Differently, van Dillen et al. (1999) observed a transition from tensile to compressive stress in alkali-borosilicate glass samples irradiated by MeV Xe ions. For high surface mobility films, it was observed that the evolution of the residual stress typically occurs in alternating stages of compressive, tensile, and compressive growth (Abermann, 1990; Floro et al., 2001; Shull and Spaepen, 1996; Spaepen, 2000), exhibiting a rather complicated stress generation mechanism.

Motivated by these experimental observations, predicative theoretical models have been developed to study stress generation mechanisms during ion irradiations. Within the framework of elasticity, Guinan (1974) obtained a rough estimate of thermal stress induced by a single impinging ion in terms of the dissipated energy in the damage zone. It is however not straightforward to extend this model to the cases where many energetic ions sequentially impact the substrate since the existing damage regions may have a strong influence on the subsequent defect production. Based on the knock-on linear cascade theory, Windischmann (1987) predicted a square-root dependence of compressive stress on the incident ion energy. This model, however, is not applicable to cases of high incident energy. Davis (1993) and Robertson (1993) separately developed a subplantation model in which the compressive stress formation in thin films is attributed to densification of subsurface due to ion implantation. An underlying assumption of the subplantation model is that the film surface, upon ion bombardment, is overdense containing no voids. However, experimental measurements and numerical simulations indicate that films are usually under-dense. For epitaxially grown thin films on a substrate, it has been well established that the lattice-mismatch is the driving force for the thin film surface stress (Freund and Nix, 1996). Stress evolution during film growth has also been attributed to competing mechanisms between island growth and coalescence (Floro et al., 2001; Nix and Clemens, 1999). For polycrystalline films, Chason et al. (2002) developed a model of stress evolution during film growth, in which the generation of compressive stress in the films is attributed to the flow of excess atoms into grain boundaries driven by surface chemical potential due to the impinging growth flux.

Molecular dynamics (MD) simulations have been carried out to uncover the stress generation mechanisms during ion irradiations (Gibson et al., 1960; Jager and Albe, 2000; Kalyanasundaram et al., 2006; Kaukonen and Nieminen, 1992; Kaukonen and Nieminen, 2000; Kinchin and Pease, 1955; Marks et al., 1996; Muller, 1987; Zhang et al., 2003). Depending on the substrate materials and the kinetic energy of the incident ions, the generated stress can be either compressive or tensile. These MD simulations allow direct investigation of the atomic structures of the surface region impacted by energetic ions. Results of the MD simulations may provide useful insight into the atomistic mechanisms of stress generation. For example, for only a few ion bombardments, Gibson et al. (1960) observed that the damaged configuration primarily consists of interstitial–vacancy pairs, i.e., the Frenkel defects. Muller (1987) found that ion-irradiated nickel films contain a