Computational Materials Science 149 (2018) 230–242

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

The mechanism of plastic deformation in intact and irradiated GaN during indentation: A molecular dynamics study

Yu Qian[a], Fulin Shang[a,*], Qiang Wan[b], Yabin Yan[b]

[a] State Key Laboratory for Strength and Vibration of Mechanical Structures, School of Aerospace, Xi'an Jiaotong University, Xi'an 710049, Shaanxi, PR China
[b] Institute of System Engineering, China Academy of Engineering Physics, Mianyang 621900, Sichuan, PR China

ARTICLE INFO

Keywords:
Molecular dynamics
GaN
Plastic deformation
Indentation

ABSTRACT

A series of molecular dynamics simulations are carried out to study the mechanical properties of GaN. Firstly, indentation simulations are performed on the *c*-plane and *m*-plane GaN. Combined with the evolution of defects in the GaN substrate, the anisotropic mechanical responses are discussed in detail. It is found that plastic deformation in an intact *c*-plane GaN starts with generation and extension of planar defects. These planar defects eventually gather together and transform into a disordered region with a growing size. While for the *m*-plane GaN, the deformation during an indentation is dominated by the nucleation and propagation of dislocations. Secondly, the irradiation effect on the mechanical properties of GaN is investigated. Irradiated models, which subjected to different irradiation dose ranging from 5 eV/atom to 50 eV/atom, are adopted in the indentation simulations. A hardening phenomenon is found for the low-dose irradiated *m*-plane GaN, and the hardnesses of *c*-plane and *m*-plane GaN decrease significantly when the irradiation dose exceeds 30 eV/atom. In addition, the indentations conducted on the irradiated models induce dramatically different deformation behaviors. In particular, with the increase of irradiation dose, the deformation mechanism transforms from the plastic activities on slip systems to local rearrangements of atoms in disordered regions.

1. Introduction

As a direct wide band gap semiconductor, gallium nitride (GaN) has attracted considerable interests for a wide range of applications in optical, high-power and high-frequency devices [1–4]. In most optical-electronic devices, the GaN material is typically in the form of a *c*-plane (0 0 0 1) film, and the *c*-plane wurtzite heteroepitaxial crystal growth on substrates such as sapphire is a mature technology [5,6]. However, epitaxial growth of GaN in *c*-direction [0 0 0 1] leads to spontaneous and piezoelectric polarization which might negatively affect the performance of devices. In order to eliminate polarization in the electric field, fabricating the GaN material on a nonpolar crystal plane has been employed, and the stable *m*-plane (1 0 −1 0) GaN has been commercially available at present [7–9].

A comprehensive understanding of the mechanical property of GaN is crucial and necessary in designing and producing the semiconductor devices, since material is subjected to unavoidable contact loads through the fabrication and encapsulation of GaN devices. And the damage caused by mechanical loads can significantly degrade the performance of the GaN devices. In addition, there is a trend that the dimensions of optical- and electrical-devices are becoming smaller. When the size of a device deceases to the micro/nano-scale, the mechanical behavior would even cause great influence on the stability of device. Persistent efforts have been made to investigate the mechanical characteristics of GaN using depth-sensing indentation tests [10–23]. Most of the indentation researches focus on the *c*-plane GaN, while little discussion has been conducted on the mechanical property of *m*-plane GaN. Besides, some of the experimental conclusions about the deformation behavior of GaN are ambiguous and inconsistent. Through the investigation on the indented surface of the specimen, Weyher [18] proposes that the slip systems on the *m* planes {1 0 −1 0} and *c* planes {0 0 0 1} are invoked during the indentation. While according to other experimental reports by Bradby [19], Jian [21], and Huang [22], the plastic deformation of *c*-plane GaN is primarily due to the slips on both *c* planes {0 0 0 1} and *s* planes {1 0 −1 1}. Fujikane [23] observes the nucleation of slips on the *c* planes {0 0 0 1}, *m* planes {1 0 −1 0}, and *r* planes {−1 0 1 2} in an indentation conducted on the *m*-plane GaN, and the experimental results manifest that the slip system firstly activated is {−1 0 1 2}⟨−1 0 1 1⟩. Hence, though it has been confirmed that the plastic deformation of GaN film in an indentation is dominated by nucleation and multiplication of dislocations on slip planes, further research is still necessary to reveal the accurate deformation

* Corresponding author.
E-mail address: shangfl@mail.xjtu.edu.cn (F. Shang).

https://doi.org/10.1016/j.commatsci.2018.03.041
Received 9 January 2018; Received in revised form 18 March 2018; Accepted 19 March 2018
0927-0256/ © 2018 Elsevier B.V. All rights reserved.

mechanism of GaN.

Another issue of interest is the irradiation effect on the mechanical behavior of GaN. Ion beam implantation, which implants dopant atoms into material and consequently alters the material properties, is an useful tool for design and fabrication of GaN-based devices. However, the inevitable implantation induced damage in lattice has not been efficiently controlled yet. Extensive experimental studies on the damage buildup in GaN under the ion bombardment have been made [24–27], and it is suggested that irradiation induced amorphization would be influenced by many conditions such as the mass of dopant atom, ion energy, implantation temperature, and beam flux. Moreover, there is considerable interest in determining the influence of ion implantation on the mechanical property, since it is the prerequisite for the successful application of implanted GaN [26,28–30]. The ion bombardment dramatically modifies the mechanical properties of GaN. For example, the amorphized GaN is much softer than the intact GaN, and there is no dislocation nucleated in the indentation of amorphized GaN, which is not alike with that of crystalline GaN. The deformation mechanism at atomic scale remains to be further studied.

In the present work, the deformation mechanism of wurtzite GaN is studied using molecular dynamics (MD) simulation. Firstly, indentation simulations are performed on the *c*-plane and the *m*-plane (0 0 0 1) surfaces of an intact wurtzite GaN. The deformation behavior is discussed in detail by studying the relation between the load-depth curves and the defect evolution in the material. Secondly, irradiated GaN models are prepared by following a two-phase iteration scheme proposed by Nord [31,32]. Then a series of *c*-plane and *m*-plane indentation simulations are carried out to examine the irradiation effect on the deformation mechanism.

2. Methodology

2.1. Interatomic potential

The indentation system was consist of a diamond indenter and a wurtzite GaN substrate. Hence the interactions between Ga, N, and C atoms were considered. We adopted a Tersoff-Berenner bond-order potential for Ga-Ga, N-N, and Ga-N, since this potential could accurately reproduce the structural and mechanical properties of GaN [33,34]. In order to achieve a reasonable response of contact loading and to reduce the computational cost, the Lennard-Jones potential was chosen to describe the interactions of C-Ga and C-N,

$$E = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], \quad r < r_0 \tag{1}$$

where r is the distance between two atoms; σ and ε are potential parameters for equilibrium distance and cohesive energy, respectively. These potential parameters were calculated according to the long-range Vander Waals interaction [35], and their values are listed in Table 1.

Besides, in the irradiation simulation, the Ziegler-Biersack-Littmark (ZBL) universal repulsive potential was smoothly jointed to the Tersoff potential to describe the interaction between the high energy atoms at short interaction distance [31,32].

2.2. Simulation model

Fig. 1 shows the unit cell structure of wurtzite GaN. From a preliminary calculation by the MD method, we had determined the unit cell parameters of a, b, c, and u which gave the minimal total energy E for a wurtzite GaN. A cubic GaN substrate with a dimension of about 20 nm × 20 nm × 20 nm was constructed. And nanoindentation simulations were performed on the *c*-plane and *m*-plane surfaces of the wurtzite GaN crystal, respectively. In each simulation, periodic boundary conditions were applied in the two directions perpendicular to the indent direction. Three bottom atomic layers were fixed to prevent the substrate from shifting. The simulation system was sufficiently relaxed, and the temperature was kept at 0 K by the Nose-Hoover method. An NPT ensemble was adopted in the indentation simulations using a time integration step of 1 fs.

Table 1
Lennard-Jones potential parameters for C-Ga and C-N.

Parameters	C-Ga	C-N
σ, equilibrium distance (Å)	3.6919	3.3677
ε, cohesive energy (meV)	8.4646	3.7235

It was well accepted that the choice of the indenter was important for an indentation and depended upon the information one wanted to obtain from the test, since different mechanical responses and deformation behaviors would be induced according to the shapes of different indenters [36]. Spherical indenters, which offered a gradual transition from elastic to elastic-plastic contact, had been usually adopted in researches on the ceramics, and robust results were achieved [37–44]. Nevertheless, if an indenter with a sharp tip or steep edges was adopted, stress in the material would firstly concentrate at the region which contacted the tip or the edges of the indenter during penetrating, which result in the plasticity around the concentrated stress. For a wurtzite GaN, the slip planes were classified as the basal plane ({0 0 0 1}), the prism planes ({1 0 −1 0}, {1 1 −2 0}), and the pyramidal planes ({1 1 −2 2}, {1 1 −2 1}, {1 −1 0 1}, {1 −1 0 2}). In view of the slip planes, a cubic indenter, which was constructed in the diamond lattice with a flat square cross section of 40 Å × 40 Å, was intentionally set up in our simulations. More concretely, as shown in Fig. 2(a), for the indentation on the *c*-plane GaN, the indenter was oriented so that the bottom edges were parallel to the [1 0 −1 0] and [−1 2 −1 0] directions. While for the *m*-plane indentation model, the orthogonal edges of the indenter bottom followed the [0 0 0 −1] and [−1 2 −1 0] directions. Thus, in the *c*-plane indentation, the concentrated stress around the [−1 2 −1 0] indenter edges would activate plastic slips on the {1 0 −1 2}, {1 0 −1 1}, or {1 0 −1 0} planes. While the stress at the [1 0 −1 0] edges would induce plastic slips on the {−1 2 −1 2}, {−1 2 −1 1}, or {−1 2 −1 0} planes. Similarly, in the *m*-plane indentation, slips on the {−1 2 −1 0}, {1 0 −1 0}, {0 0 0 1}, {1 0 −1 1}, or {1 0 −1 2} planes would be activated by the stress concentrated around the orthogonal edges of the indenter. Consequently, plastic slips would be activated more directly. In addition, all the possible scenarios of plasticity were considered in the indentations conducted on the *c*-plane and *m*-plane GaN.

A quasi-static loading method was adopted, i.e. the indenter was displaced 0.1 Å along the indent direction after every holding stage of 500 time steps. As a result the indenter penetrated into the GaN substrate at a velocity of 20 m/s by 15 Å. The load was calculated as the indent-direction component of the force exerted on the indenter. And the penetration depth was calculated as the distance between the indenter bottom and the substrate surface.

Irradiated GaN models were generated by reproducing the simulation of successive 5 keV recoils in an intact crystal. A two-phase iteration scheme proposed by Nord was adopted to model the continuous irradiation, such method had been successfully applied to simulate the amorphization process in Si, Ge, GaAs, and GaN [31,32]. In the first phase, an energetic recoil was started from the center of the cell. The primary knock-on atom (PKA) was generated by giving a random Ga atom or N atom 5 keV of kinetic energy. The cell was cooled down towards 0 K at the borders using Berendsen temperature control method, and the volume of the crystal was not allowed to change. A variable time step was employed in case of overlapping atoms and to speed up the simulation. In the second phase, the cell was sufficiently relaxed. To be specific, the system was further cooled down to 0 K, meanwhile, the pressure was relaxed with Berendsen method to 0 kbar in all directions. After the relaxation phase, atoms in the cell were displaced by a random distance in the x, y and z directions, and the

Download English Version:

https://daneshyari.com/en/article/7957574

Download Persian Version:

https://daneshyari.com/article/7957574

Daneshyari.com