Superlattices and Microstructures xxx (2017) 1–6

Contents lists available at ScienceDirect

Superlattices and Microstructures

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

Structural properties and defects of GaN crystals grown at ultra-high pressures: A molecular dynamics simulation

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ARTICLE INFO

Article history:
Received 29 October 2017
Accepted 26 November 2017
Available online xxx

Keywords:
Crystal defects
Structural properties
Liquid GaN
Coherent twin boundaries

ABSTRACT

The growth of GaN crystals at different pressures was studied by molecular dynamics simulation employing the Stillinger–Weber potential, and their structural properties and defects were characterized using the radial distribution function, the Voronoi polyhedron index method, and a suitable visualization technology. Crystal structures formed at 0, 1, 5, 10, and 20 GPa featured an overwhelming number of <4 0 0 0> Voronoi polyhedra, whereas amorphous structures comprising numerous disordered polyhedra were produced at 50 GPa. During quenching, coherent twin boundaries were easily formed between zinc-blende and wurtzite crystal structures in GaN. Notably, point defects usually appeared at low pressure, whereas dislocations were observed at high pressure, since the simultaneous growth of two crystal grains with different crystal orientations and their boundary expansion was hindered in the latter case, resulting in the formation of a dislocation between these grains.

1. Introduction

Gallium nitride (GaN), a promising wide-bandgap III–V semiconductor with excellent physical and chemical properties [1], finds extensive applications in optoelectronic [2], high-temperature/high-power [3], and high-frequency microwave devices [4,5]. Recently, one-dimensional GaN nanowires have also attracted much interest as promising materials of optoelectronic nanodevices [6–8].

Currently, the preparation of solid GaN has been extensively characterized, e.g., it was shown that the growth pressure influences the surface roughness of epilayers and their crystal quality. Importantly, growth at 200 mbar was most suitable for the preparation of high electron mobility transistors with a 1.7-μm-thick GaN buffer layer [9]. At the lower initial growth pressure, the dislocation-induced scattering was dominant especially at temperatures below 200 K, which was inessential for the higher initial growth pressure. Hall effect measurements indicated that overgrown Si-doped GaN layers formed at higher initial growth pressures exhibit higher mobility [10]. Whereas another study determined the effects of growth pressure (100–400 mbar) on the properties of *p*-GaN prepared by low-temperature metalorganic chemical vapor deposition [11].

In contrast to experimental methods, computer simulation enables the effective investigation of microstructures for a better understanding of their physical and chemical properties. Thus, the interatomic potential, a bond order potential developed for GaN, exactly reflects certain structural and material properties of Ga, N, and GaN, including defects and multiple crystal phases [12]. Moreover, the physical properties of Ga–N systems can be studied using an empirical potential (e.g., the Tersoff potential)

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https://doi.org/10.1016/j.spmi.2017.11.054
0749-6036/

in combination with molecular dynamics (MD) methods [13]. Additionally, some researchers used the Buckingham potential parameters for wurtzite, zinc-blende, rock-salt, and NiAs structures of GaN, successfully calculating the dynamical properties of the above semiconductor under pressure [14]. Compared to those of numerous hexagonal closed-packed metals, the computed dislocation mobility in GaN was low but still finite, as exemplified by the mobilities and anisotropy of three *a*-type $[1\ \ 1\ \ \bar{2}\ \ 0]$ threading edge dislocations in wurtzite GaN determined by classical MD simulation [15].

However, although structural information on point defects and dislocations is needed for the development of next-generation high-quality materials, quantitative analyses of locally ordered structures in GaN are still scarcely reported, especially the structural properties at ultra-high pressure. Herein, we utilized MD simulation and the Stillinger–Weber (S–W) potential [16] to study the crystal growth of GaN during rapid solidification at different pressures and the structural properties of the thus formed defects. The above potential is suitable for tetrahedral semiconductors such as Si, Ge, and GaN [17]. The radial distribution function (RDF) [18] was used to characterize the formation and evolution of crystal structures, and the effect of pressure on microstructures was investigated in detail using Voronoi polyhedron indices [19,20], with the evolution of crystal structure and defects revealed using a suitable visualization technology.

2. Simulation conditions and methods

MD simulations were carried out in a cubic box and subjected to widely used periodic boundary conditions with 8000 atoms (4000 Ga atoms and 4000 N atoms). Simulations were conducted in the NPT (with constant atom number, system pressure and temperature) ensemble at a cooling rate of 10^{11} K/s and a time step of 1.0 fs. The initial configuration featured equilibration at 300 K in 200,000 time steps, with several successive equilibrations subsequently simulated by increasing the temperature in 200-K steps, which were decreased to 50 K upon approaching the melting temperature of GaN. The system completely melted at 4600 K and was further simulated for 100 ps to guarantee the formation of an equilibrium liquid state based on its total energy and microstructures. In the next stage, the melt was subjected to pressures (p) of $P_0 = 0$ GPa, $P_1 = 1$ GPa, $P_5 = 5$ GPa, $P_{10} = 10$ GPa, $P_{20} = 20$ GPa, and $P_{50} = 50$ GPa, and the temperature was gradually decreased to 200 K at a cooling rate of 10^{11} K/s. For structural property analysis, information on all atoms during quenching was recorded at every 50 K. Finally, several structural characterization methods were used to analyze the crystal structures of GaN grown at different pressures and the corresponding defects.

3. Results and discussion

3.1. Radial distribution function

The RDF describes how density varies as a function of distance from a reference particle in a given system, being widely used to reveal the structural characteristics of liquids and amorphous solids. To understand the atomic arrangement of GaN during quenching, g(r)s was recorded at several pressures (Fig. 1). The obtained results revealed that crystalline structures

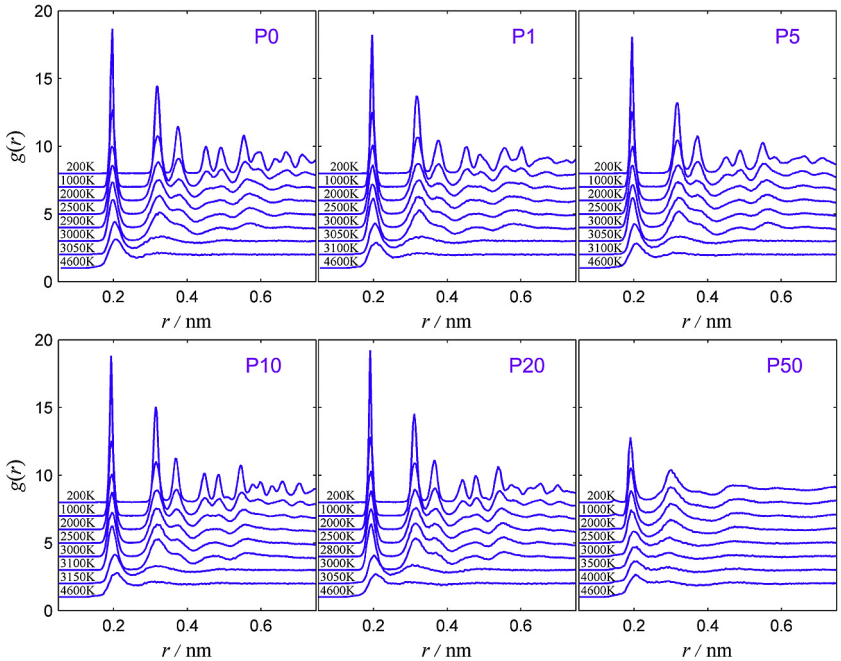

Fig. 1. RDF evolution at different pressures during quenching. ($P_1 = 1$ GPa, $P_5 = 5$ GPa, $P_{10} = 10$ GPa, $P_{20} = 20$ GPa, and $P_{50} = 50$ GPa).

Please cite this article in press as: T. Gao et al., Structural properties and defects of GaN crystals grown at ultra-high pressures: A molecular dynamics simulation, Superlattices and Microstructures (2017), https://doi.org/10.1016/j.spmi.2017.11.054