Molecular dynamics simulations of GaAs-crystal surface modifications during nanoindentation with AFM tip.

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Abstract. The nanoindentation model of atomically flat surface of GaAs with the AFM tip was developed on the base of Molecular Dynamics. It was found that as a temperature rises above 100 K the nanoindentation results in increase of number of atoms with higher number of neighbours, i.e. point defect appears in the topmost atomic layers of GaAs. The observed results can be explained with the kinetic concept of the mechanism of fracture of solid state where the generation of native point defects caused by the fluctuation of thermal energy and the external stress results in enhancement of the defect generation rate.

1. Introduction

Tribological phenomena occur by mechanical interaction of sliding surfaces during their relative motion. Important role in this process is played by the individual multiple point contacts between the rubbing surfaces, whose total area is much smaller than would follow from the geometrical sizes of contacting parts. At the initial stage of the development of tribology, the main tasks were primarily of an engineering nature, since they were associated with the study of the properties of macroscopic contacts of details of various mechanisms. Many specific tribological problems, cannot be solved analytically, therefore, numerical simulation methods in the mechanics of contact interaction and friction physics are needed. Tribological study have reached a new level with the invention of atomic force microscopy (AFM) technique, when there was an opportunity to explore (with high spatial resolution) physical properties of a single point nanocontact, formed between an apex of AFM tip and the sample surface. It was found that the physical processes in nanotribology are much broader and include many new phenomena, such as phase transitions caused by shear ordering of thin films in tip-surface contact, chemical effects associated with moisture, superconductivity, electrochemical and triboelectric effects, etc [1].

One of the main instruments of nanotribology is molecular dynamics (MD) simulations, which makes it possible to move from mechanics of continuous media to atomistic modeling [2, 3]. MD is based on classical dynamics, where atoms are represented as points of mass interacting with each other according to interatomic potentials. The trajectories of atoms and molecules are determined by numerical solution of Newton's equations of motion for a system of interacting particles, where the forces between particles and the potential energy are determined by interatomic potentials.

Recently, the process of triboelectrization of atomically flat epitaxial n-GaAs layer after scanning by AFM tip in contact mode was studied [4, 5]. The surface of GaAs (001) epitaxial layers grown by MOCVD technology was selected as the test object with a high crystalline quality of the both surface and bulk. Changes in local surface potential of these samples after treatment with the AFM tip was explained by nanotribological generation of native point defects in a few atomic layers below the GaAs surface. They produce additional energy states within the GaAs bandgap. Free electrons can be captured...
on the surface states, which results in additional negative charge on the surface and decreasing its potential [4, 5].

This work presents results of the MD simulations of nanoindentation process of atomically flat GaAs surface with the apex of AFM tip, as a function of temperature.

2. Details of simulation

The MD calculations were carried out using the LAMMPS Molecular Dynamics Simulator [6]. To describe the atomic interaction in GaAs sample with a perfect crystalline structure we used the bond-order potential (BOP), based on quantum mechanical theory incorporating both σ and π bonds [7]. The GaAs slab has the following parameters: height is 12 nm, depth and width are 56 nm each. The simulated GaAs slab consists of 1,700,000 atoms. The bottom monomolecular Ga-As layer is fixed. The orientation of the top surface of GaAs is (001) plane. The MD simulation was carried out with the periodic boundary conditions for vertical planes at the edges of the GaAs slab. The atomic system was described as canonical (NVT) ensemble, which means constant number of atoms, volume and temperature. Discretization time in MD simulations is 10 fs.

The apex of the AFM tip is modelled as absolutely rigid nanoindentor based on semisphere with radius of 10 nm. The normal velocity of nanoindentor is 1 m/s. During MD simulations the indenter moves with a constant velocity into the top surface of the GaAs slab and stops at the depth of 1 nm, where it stays until the end of the simulation process. The modeling of the nanoindentation process was carried out without lateral movement of the indenter. Also the action of capillary and adhesion forces was neglected.

3. Results and Discussions

Figure 1 represents 2D distribution of the $\varepsilon_{zz}$ component of Green-Lagrangian strain tensor [8] calculated at temperature 10 K with nanoindentation depth of 0.5 nm (Fig. 1a) and 1.0 nm (Fig. 1b). At a depth of indentation of 1 nm the most strained region is located at the depth of 1.5 nm under the indenter (Fig. 1b). This indicates the most probable region of point defect generation. Even at maximum indentation depth of 1 nm there are no any signs of surface destruction under the indenter at temperature 10 K (Fig. 1b). The normal force applied in this case can be calculated on the base of Hertz approach which describes the contact between the inelastic ball with the elastic surface [9]. For the nanoindentation process it gives the normal force of 90 nN at the depth of 0.5 nm and 280 nN at the depth of 1.0 nm.

![Figure 1](image)

**Figure 1 (a,b).** 2D distribution of the $\varepsilon_{zz}$ component of Green-Lagrangian strain tensor (indicated by colour) calculated at temperature 10 K with nanoindentation depth of 0.5 nm (a) and 1.0 nm (b).

We also performed the MD simulation for different temperatures in the range from 10 K to 900 K (Fig. 2a, b). The strained region still exist at the depth of 1.5 nm below the surface, but it becomes blurred with an increase of temperature. But nevertheless the appearance of the strained area is still noticeable. It is worth to note the MD simulations shows that at temperatures above 100 K the nanoindentation to the depth of 1.0 nm results in formation of point defects in the 2-3 topmost atomic layers (Fig. 2a, b). And these defects do not disappear after release of the nanoindentor. To estimate the
point defect concentration we calculated the number of atoms \( N_S \) located under the indenter within the cylinder with the diameter of 6.4 nm and the depth of 10 monolayers as a function of number of nearest neighbors of one atom within a cutoff radius of 3 Å (Fig. 3). For a perfect GaAs crystal the typical number of neighbors is 4 for the atoms in the bulk and 2 or 3 for atoms located at the surface. The MD simulation at the indentation depth of 1.0 nm carried out at temperature 10 K shows no any defects in topmost atomic layers under indenter (Fig. 1a, Fig. 3). As a temperature rises the nanoindention results in increase of number of atoms \( N_S \) with higher number of neighbours, i.e. point defect appears in the topmost atomic layers of GaAs (Fig. 3).

![Figure 2 (a,b) 2D distribution of the \( \varepsilon_{zz} \) component of Green-Lagrangian strain tensor (indicated by colour) calculated with nanoindentation depth of 1.0 nm at temperature 300 K (a) and 900 K (b).](image)

![Figure 3. The number of atoms \( N_S \) located under the indenter as a function of number of nearest neighbors at different temperatures. The depth of indentation is 1 nm.](image)

The results could be explained using the kinetic concept of the mechanism of fracture of solid state [10]. It is based on two statements that the driving force of the fracture of solids is the fluctuation of thermal
energy and the external stress induces enhancement of the rate of thermal production of point defects. The external force does not directly break the interatomic bonds, but only prevents the restoration of broken bonds.

4. Conclusions
The nanoindentation model of atomically flat surface of GaAs with the AFM tip was developed on the base of Molecular Dynamics. The distribution of the $\varepsilon_{zz}$ component of Green-Lagrangian strain tensor was calculated at different temperatures. It was found that at temperature 10 K indentation up to the depth of 1.0 nm shows no any defects in topmost atomic layers under indenter. As a temperature rises the nanoindentation results in increase of number of atoms with higher number of neighbours, i.e. point defect appears in the topmost atomic layers of GaAs. The observed results can be explained with the kinetic concept of the mechanism of fracture of solid state where the generation of native point defects caused by the fluctuation of thermal energy and the external stress results in enhancement of the generation rate. The findings allow to explain the observed earlier the experimental results on modification of surface potential of GaAs after the scanning with the AFM tip.

Acknowledgments
This study was supported in part by the Russian Foundation for Basic Research, project no. 15_01_05903.

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