Elastic Stress Relaxation in the AlN/SiC Heterostructures: Modeling by Utilizing the Molecular Dynamics Method

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Abstract: A computer study of crystallographic features of lattices detected near their heterogeneous boundaries was performed within the general direction of research on the AlN/SiC heterostructures considered as a promising platform for functional electronics intended to operate under extreme temperature conditions (including volcano research, geyser monitoring, ultradeep drilling, etc.). Modeling by means of the molecular dynamics method utilizing the Tersoff potentials (for SiC) and the potential proposed by Vashishta (for AlN) allowed researchers to obtain a 3D description of the energy landscape and locations of its characteristic points (minima, saddle points). Minimizing the total crystallite energy as the lattice configuration varies with changes in the distance from the interface makes it possible to directly calculate the characteristic relaxation length in the elastic stress field posing a direct interest for the technology of low-defect nanolayers.

1 INTRODUCTION

Giant hydrothermal systems formed in the areas of magmatic activation of the earth's crust are of interest not only from their huge geothermal potential point of view, but also as convenient objects for seismic activity monitoring. The significance of such fractured-porous geological structures, formed at depths up to 10kM and filled with hot mineral solutions and superheated dry steam at a high pressure, is not least due to their relatively high prevalence. Suffice it to mention such hydrothermal formations as Geysers (USA, California), which go to a depth of ~8kM and have a temperature of up to 700ºC (Walters, et al., 1992); Larderello (Italy) has temperatures up to 420ºC and is characterized by high temperature gradients (Bellani, et al., 2004); systems Wayang Windu (Indonesia) with a significant reserve of geothermal energy (Bogie, et al., 2008); Hohi and Sengan, Japan (Tamanyu, et al., 1991) or Ebeko volcano, Russia (Rychagov, et al., 2010).

Since the local parameters of such geothermal systems largely characterize the seismological state of the region and allow to make the necessary forecasts or contribute, for example, to the development of sound recommendations for the construction of geothermal power plants, it seems timely to carry out work aimed at creating a distributed monitoring system based on deep high-temperature sensors of the environment thermodynamic and chemical state.

2 PROBLEM STATEMENT

The creation of reliable and thermally stable sensors capable of operating for a long time in a high-temperature and aggressive environment is possible only when using wide-band semiconductor or functional materials such as silicon carbide (SiC) and aluminum nitride (AlN), which, among other attractive properties, are distinguished by exceptional chemical resistance, mechanical strength and thermal stability of parameters (Fraga, et al., 2014). Currently, SiC is the main candidate for creating the element base of high-temperature electronics, and microcircuits have already been created for operation in the range of up to 500ºC (Tian, et al., 2017; Kargarrazi, et al., 2018; Spry, et al., 2018), while AlN is a functional material, on the basis of which it is possible to create pyrosensors, strain gauges and chemical sensors (Gavrilov, et al., 2018; Umeda, et al., 2013; Jiang, et al., 2014).

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. In addition, advances in modern epitaxial technologies make it possible to obtain SiC/AlN heterostructures (Panyutin, et al., 2020), which opens the way to single-chip integration of an AlN sensor with a high-temperature SiC microcircuit capable of performing primary processing of an analog signal and representing it in digital form.

However, the absence of an exact match between the crystallographic parameters of these materials leads to the appearance of an elastically stress, which is usually maximum at the heterointerface and gradually decreases as it moves away. The purpose of this study is to determine the nature of the relaxation of this elastic stress within the framework of the molecular dynamics method, which is of practical importance for the technology of nanolayered heterostructure.

3 MODELING

Classical molecular dynamics method is one of the effective computational approaches, within which many of the topical problems of this kind can be solved.

The main idea of this method is to describe a spatially ordered set of N atoms with coordinates r_i, each of which interacts with all the others through a certain type of potential $U(r_i-r_j)$, depending on the pairwise distances between these atoms or ions and representing curves with a minimum that determines their thermodynamically stable configuration. With regard to crystalline structures, only the total (multi-particle) potential, which is a superposition of partial potentials corresponding to the interaction of arbitrary pairs of atoms, has real physical meaning.
For semiconductor crystals, which are characterized by the predominance of the covalent contribution to interatomic bonds, Tersoff's multiparticle potentials (Tersoff J., 1988), which are based on the mathematical formalism for systems with ordered bonds proposed by Abel (Abell, 1985), seem to be preferable.

In a somewhat simplified form, it can be represented as follows:

$$V(x,y,z)=\frac{1}{2}\sum_i V_i=\frac{1}{2}\sum_i \sum_{j\neq i}\phi(r_{ij}) \quad (1)$$

Here V_i is the energy of an atom of the i-th lattice site, $\Phi(r_{ij})$ is the energy of interaction between atoms i and j belonging to this lattice and located at distances $r_{ij}=(x_{ij}^2+y_{ij}^2+z_{ij}^2)^{1/2}$, and it is assumed that this energy depends on the simultaneously acting attraction and repulsion forces and is determined by the expression:

$$\phi(r_{ij})=f_c(r_{ij})\left[\phi_{rep}(r_{ij})+b_{ij}\phi_{att}(r_{ij})\right] \quad (2)$$

In this case, the function $\Phi_{rep}(r_{ij})$ is a repulsive pair potential determined by the interaction of electron shells at short distances, as well as the interaction of nuclei, and the function $\Phi_{att}(r_{ij})$ is an attraction potential, and includes the forces of covalent attraction of outer electron shells.

$$\phi_{rep}(r_{ij})=A_{ij}\exp(-\lambda_{ij}r_{ij}) \quad (3)$$

$$\phi_{att}(r_{ij})=-B_{ij}\exp(-\mu_{ij}r_{ij}) \quad (4)$$

$$f_c(r_{ij})=\tfrac{1}{2}+\left(\tfrac{1}{2}\right)cos\left[\pi\cdot\psi\right] \quad (5)$$

Here ψ is the angle between the directions of bonds between the i-th and j-th atom; λ, μ are the scale factors obtained from the values of elastic constants. The numerical values of the parameters for SiC can be found in (Le, et al., 2014). The potential that is reasonable to use for AlN was first proposed by Vashishta (Vashishta, et al., 2007). It combines repulsive, charge-dipole, Coulomb with screening and dispersion interactions and has been successfully used for a number of $A^{III}B^{V}$ semiconductors.

The potential can be represented (Henggao Xiang, et al., 2017) as:

$$V=\sum_{i<j}V_{ij}^{(2)}(r_{ij})+\sum_{i,j<k}V_{ijk}^{(3)}(r_{ij},r_{ik}) \quad (6)$$

$$V_{ij}^{(2)}(r)=\frac{H_{ij}}{r^{\eta_{ij}}}+\frac{Z_iZ_j}{r}e^{-\frac{r}{\lambda}}-\frac{D^{ij}}{r^4}e^{-\frac{r}{\xi}}-\frac{W_{ij}}{r^6} \quad (7)$$

Equation (6) generally describes two-particle and three-particle interactions, where r_{ij} are the distances between i- and j- atoms. In equation (7) H_{ij} and η_{ij} are the magnitude and index of the decay of repulsive forces, Zi is the effective charge, W_{ij} and D_{ij} represent, respectively, the constants of dipole and van der Waals interactions. The values of the parameters for this potential are given, for example, in (Henggao Xiang, et al., 2017). The calculated potential values for SiC (hexagonal lattice, *P6₃/mc* group) and AlN (hexagonal lattice of the sphalerite type), corresponding to equilibrium states, reach their minima, at lattice constants, respectively, $\boldsymbol{a}_{\infty SiC}$=3, 07 A and $\boldsymbol{a}_{\infty AlN}$= 3,11A. However, at the SiC/AlN interface, in the approximation of the absence of misfit dislocations, we can determine $\boldsymbol{a}_{0\ SiC}=\boldsymbol{a}_{0\ AlN}\approx 3,09$ A. The atomic configuration of a fragment of such an elastically stressed SiC/AlN heterostructure (a view from the YZ and XZ planes) is shown in Figure 1.

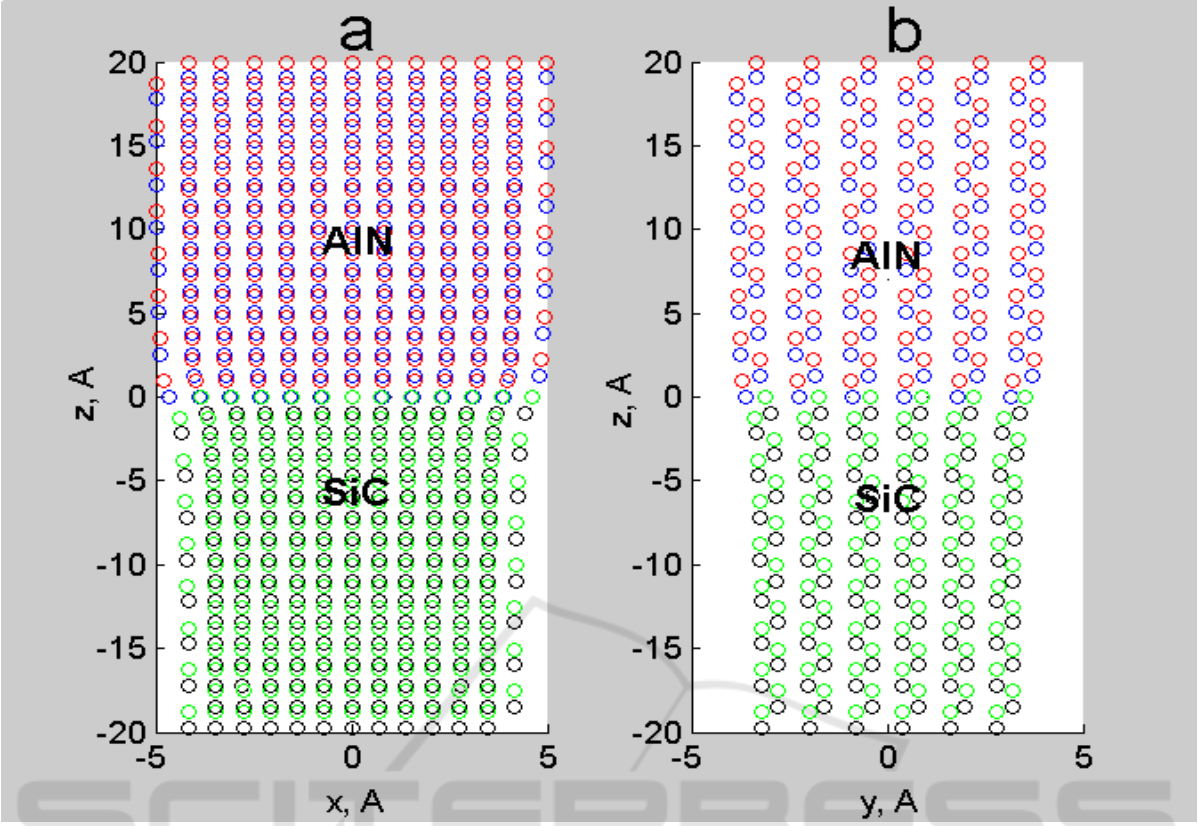

Figure 1: Atomic configuration of a fragment of an elastically stressed SiC/AlN heterostructure, a) – view in the Y direction (XZ plane), b) - view in the X direction (YZ plane)

Then, assuming that the asymptotic behavior of the lattice constants relaxation to their equilibrium values corresponds to a power law, the change in the ***a*** parameter along |z| coordinate can be represented as:

$$a_{SiC}(z) = \frac{(\Delta a_{SiC})}{(1+z^{\beta})} \quad (8)$$

$$a_{AlN}(z) = \frac{(\Delta a_{AlN})}{(1+z^{\beta})} \quad (9)$$

where $\Delta_{\boldsymbol{a}SiC}+\Delta\boldsymbol{a}_{AlN}=|\boldsymbol{a}_{\infty\ SiC} - \boldsymbol{a}_{\infty\ AlN}|$, and β are relaxation parameters.

Obviously, the equilibrium configuration of such a deformed (dislocation-free) lattice for the selected types of potentials will correspond to such value of β, for which the total crystallite energy V will take a minimum value. The corresponding values of the relaxation parameter β for crystallites of various thicknesses (dimension Z direction) are shown in Figure 2.

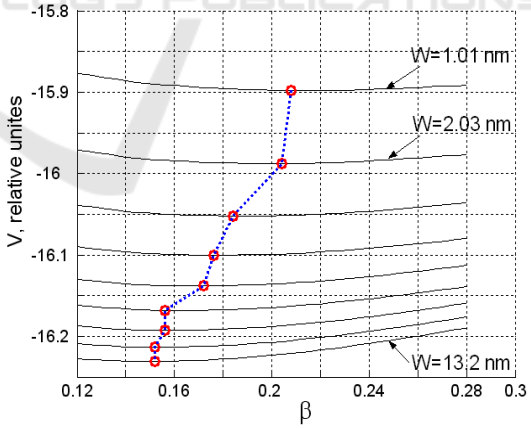

Figure 2: Dependence of the potential V of a fragment of the AlN/SiC structure on the possible values of the relaxation parameter β for various thicknesses W of the crystallite. The real values of β correspond to its value at which the potential V reaches a minimum.

All calculations were made in the MATLAB.

4 CONCLUSION

This study of the lattice parameters deviation from their equilibrium values is of great importance for the development of a number of nano-devices, and, in particular, nanolayered pyrosensors. However, taking into account that, unlike the quantum mechanical approach, the molecular dynamics method is less universal and its results depend on the chosen type of interatomic potential, they require comparison with experiment for each specific case.

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