Nanoscaled silicon carbide on silicon: a new material for optoelectronics

S.A. Kukushkin, A.V. Luk’yanov, A.V. Osipov

1Institute of Problems of Mechanical Engineering RAS, V.O., Bolshoj pr. 61, St. Petersburg, 199178 Russia
2New Silicon Technologies Ltd., Magnitogorskaya 51/3, St. Petersburg, 195027 Russia

Abstract
The new method of epitaxy of low-defect unstressed nanoscaled silicon carbide (SiC) films on silicon (Si) substrates is theoretically developed and experimentally realized in the case of the big mismatch of lattices of a film and the substrate (~20%). The method consists in the replacement of a part of atoms of the Si matrix by atoms of C with the formation of SiC molecules. The laboratory model of the operating light-emitting diode is originally obtained based on these structures.

Keyword: Silicon carbide, wide-bandgap semiconductors, epitaxy, stress relaxation

1. INTRODUCTION
The tremendous elastic stress appearing during the growth of single crystal films with the lattice parameter strongly differing from the lattice parameter of the substrate do not allow us to obtain high quality layers of new wide-bandgap semiconductors without misfit dislocations. It is assumed that the most promising of these are silicon carbide (SiC), gallium nitride (GaN), aluminum nitride (AlN), zinc oxide (ZnO), and some others. Integration of these materials into the silicon electronics plays a key role for the development of industrial technologies; therefore, it is very important to deposit epitaxial films of these materials just on silicon. However, due to the large difference in lattice parameters of Si and all the mentioned wide-bandgap semiconductors (~20%), during the ordered growth of these materials the stress energy rises. This leads to the appearance of a tremendous number of misfit dislocations in growing films and even to complete film cracking.

2. THEORY
In this work, we suggest new relaxation mechanism of the elastic energy for growing dislocation-free heteroepitaxial films. The essence of this approach, which differs from all the existing methods of film growth, is based on the idea of preliminary incorporation of point defects into the crystal lattice of the silicon host. When growing the SiC film on the Si substrate, such defects are the carbon atom C placed in the Si interstitial position and the vacancy formed as a result of removal of one of the Si atoms. If these defects are attracted to each other by the elastic interaction in the Si matrix, the resulting elastic energy caused by their incorporation into the substrate host is considerably lower than the energy of noninteracting defects. It is well known that the spherically symmetric dilatation centers do not interact with each other at all in an isotropic medium of infinite size. In this work, we show that the dilatation centers can attract to each other in substantially anisotropic media, such as the crystal with the cubic lattice symmetry, thereby considerably decreasing the total elastic energy. Such attractive centers form stable objects of a new type, namely, the elastic dilatation dipoles. We calculated the elastic energy of the system using heteroepitaxy of the SiC film on the Si substrate (Si has a cubic lattice) as the example and showed that the elastic energy can relax completely only due to the ensemble of dilatation dipoles. In order to provide the effective usage of a new relaxation mechanism of elastic energy due to the interaction of point defects, we suggest the deposition process of SiC not from the vapor phase but immediately from the matrix of the single crystalline Si substrate due to the chemical reaction between the crystalline Si and gaseous carbon monoxide CO

\[ 2\text{Si (solid)} + \text{CO (gas)} \rightarrow \text{SiC (solid)} + \text{SiO (gas)} \] (1)

We selected this reaction because of the fact that the forming gaseous silicon monoxide SiO partially carries the atoms from the Si matrix inducing vacancies in it, while gaseous carbon monoxide CO is the source of carbon atoms C arranged in atomic voids of the silicon lattice. Both Si vacancies and incorporated C atoms are the compressing dilatation centers in the cubic Si lattice and interact with each other [2] (see Fig.1).

Fig. 1. Schematic illustration of elastic dipoles in the cubic lattice of Si. Large blue balls are Si atoms, small green ones are C atoms in the interstitial positions. The strings indicate the elastic interaction between dilatation centers (vacancies and C atoms) with dipole formation.

a) sergey.a.kukushkin@gmail.com
b) andr_os@yahoo.com
Figure 2 represents the difference between the classical mechanism of thin film growth and the mechanism of epitaxy suggested here. In the first case the film grows on the substrate surface which results in enormous stress energy, whereas in the last case the film grows inside the substrate, and the attraction between point defects provide the complete relaxation of the stress energy. The merging process of vacancies after film nucleation results in the pore formation under the film [1,2].

![Schematic pattern of regular thin film growth (a) and the suggested one (b). In the second case dumbbells represent the attraction between different point defects (dilatation dipoles).](image)

3. EXPERIMENTAL AND RESULTS

To confirm experimentally the suggested relaxation mechanism of elastic energy, Si (111) substrates 35 mm in diameter were held in a vacuum furnace at $T = 1100–1300^\circ$C in the atmosphere of CO at $p = 10–300$ Pa for 5–60 min [3]. A SiC film 50–200 nm thick grew inside the Si substrate during this time. The average value of tensile elastic stresses in SiC films measured by an FLX-2320-S thin film stress measurement system is 0.5 GPa in the absence of lattice misfit and cracks [4]. Microscopic analysis revealed an almost ideal conjugation of the lattices of silicon and silicon carbide [4]. Such a low measured elastic energy with the ideal conjugation of lattices in the absence of misfit dislocations and cracks can be interpreted by the relaxation of elastic stresses due to the ensemble of dilatation dipoles.

To investigate the epitaxy of wide-gap semiconductors on silicon with the SiC buffer nanolayer and to study the prospects of their use in microelectronics, GaN based light-emitting heterostructures were grown on Si(111) substrates with deposited epitaxial SiC nanolayers (~120 nm). Such structures comprise the following sequence of layers. Initially the AlN nucleation layer was deposited on the SiC/Si template, and then the transient layer of the Al$_x$Ga$_{1-x}$N solid solution with a variable Al content from $x = 1$ to $x = 0$ along the growth direction was grown. Further, the GaN layer providing planarization of the structure surface was grown. After this, we grew the standard light-emitting diode structure containing the $n$- and p-GaN layers and the active region based on five InGaN quantum wells separated by the barrier GaN layers (Fig. 3). To prevent crack formation, the total thickness of the light-emitting diode structure was limited by 2.5 μm.

![SEM image of the light-emitting diode structure on SiC/Si template received by the method of solid state epitaxy.](image)

This structure on silicon is found to possess a high carrier mobility and a low defect content. Spectrums of photo- and electroluminescence correspond to regular ones.

4. SUMMARY

Thus, a new relaxation mechanism of elastic energy due to the formation of dilatation dipoles is put forward. Usage of this mechanism allowed us to originally grow the light-emitting diode epitaxial structure on the silicon substrate and fabricate the operating laboratory model of the light-emitting diode. The employment of this relaxation mechanism also permits us to obtain heteroepitaxial films of wide-bandgap semiconductors (such as SiC, AlN, GaN, AlGaN) on silicon without misfit dislocations and cracks having sufficient quality to fabricate many devices of microelectronics and optoelectronics.

5. REFERENCES