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LOW-DIMENSIONAL SYSTEMS AND SURFACE PHYSICS

Effect of the Chromium Layer Thickness on the Morphology and Optical Properties of Heterostructures Si(111)/($CrSi_2$ Nanocrystallites)/Si(111)

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Abstract—Growth and the optical properties of epitaxial heterostructures Si(111)/($CrSi_2$ nanocrystallites)/Si(111) based on nanosized islands of chromium disilicide ($CrSi_2$) on Si(111) were studied using low-energy electron diffraction, atomic-force microscopy, and optical reflection and transmission spectroscopy. The heterostructures with thicknesses of 0.1, 0.3, 0.6, 1.0, and 1.5 nm were formed by reactive epitaxy at a temperature of 500°C followed by the epitaxial growth of silicon at 750°C. The specific features of changes in the density and sizes of $CrSi_2$ islands on the silicon surface were determined at $T = 750$°C as the chromium layer thickness was increased. It was established that, in the heterostructures with chromium layer thicknesses exceeding 0.6 nm, a small part of faceted Cr_2Si_2 nanocrystallites (NCs) emerge into near-surface region of the silicon, which is confirmed by the data from optical reflectance spectroscopy and an analysis of the spectral dependence of the absorption coefficient. A critical size of NCs is shown to exist above which their shift to the silicon surface is hampered. The decreased density of emerging NCs at chromium layer thicknesses of 1.0–1.5 nm is associated with the formation of coarser NCs within a silicon layer, which is confirmed by the data from differential reflection spectroscopy.

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1. INTRODUCTION

Chromium disilicide ($CrSi_2$) is a narrow-gap (0.35 eV) semiconductor in accordance with theoretical calculations [1–3] and experimental data [4, 5]. It is known that, on silicon with (111) orientation, epitaxial $CrSi_2$ films grow [4–7]. Plusnin et al. [5] proposed a technique for separating a preferred orientation in $CrSi_2$ films. This technique made it possible to grow continuous epitaxial *A*-type $CrSi_2$(0001) films on Si(111) [6, 7]. In such layers, noticeable changes in the electronic structure and in the carrier scattering mechanism have been revealed and a significant increase in the mobility of majority carriers (holes) and a decrease in their concentration have been observed. These changes were related to elastic stresses that occur during epitaxial growth of *A*-type $CrSi_2$(0001) films with 30° rotation relative to the silicon lattice and with a crystal lattice misfit between Si(111) and $CrSi_2$(0001) of the order of 0.1%. The presence in *A*-type epitaxial $CrSi_2$(0001) films of a certain amount of the *B*-type $CrSi_2$(0001) phase with orientation coinciding with that of the Si(111) silicon substrate makes it impossible to grow single-crystal $CrSi_2$(0001) films and produce binary heteroepitaxial structures Si(111)/$CrSi_2$(0001)/Si(111). Such structures are of interest for silicon microelectronics and optoelectronics as photoelectrical transducers and heterostructure transistors. However, instead of continuous epitaxial $CrSi_2$(0001) films, island $CrSi_2$ films can be used with island sizes of several tens of nanometers. This approach can be used to prepare silicon with an embedded layer or layers of $CrSi_2$ nanocrystallites (NCs), which can be elastically adjusted to the silicon lattice parameters, creating a high density of $CrSi_2$ NCs/Si heterojunctions [8]. At a $CrSi_2$ NC density higher than 10^{10} cm^{-2}, hopping conduction can occur between the nanocrystallites, and this conduction will depend on the properties and defect structure of the $CrSi_2$ NCs/Si interface. This behavior of the conductivity should lead to changes in the electrical and optical properties of the heteroepitaxial structures Si(111)/$CrSi_2$ NCs/Si(111) and can also be used to design new types of apparatus structures.

In [9], we established that, upon reactive deposition of chromium on an atomically pure Si(111)7 × 7 surface at 500°C followed by epitaxial silicon growth, monolithic Si(111)/$CrSi_2$(0001) NCs/Si(111) heterostructures are formed; we also grew multilayer (2- to 6-layer) monolithic heterostructures with a silicon-layer thickness of 36 nm. However, the effect of the chromium layer thickness on the formation of nanosized