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Atomistic modeling of strain distribution in self-assembled interfacial misfit dislocation (IMF) arrays in highly mismatched III–V semiconductor materials

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Abstract

We describe a mathematical model to elucidate the strain energy distribution in the atomic arrangement resulting from a periodic pure edge, 90° interfacial misfit dislocation (IMF) arrays in highly mismatched III–V semiconductors. Using molecular mechanics methods, we calculate strain energy at the atomic level by considering the stretch and bend of each bond in the system under consideration. Three highly mismatched systems InAs/GaAs ($\Delta a_o/a_o$ ~7.2%), GaSb/GaAs ($\Delta a_o/a_o$ ~7.8%) and AlSb/Si ($\Delta a_o/a_o$ ~13%) are considered. This model describes that IMF array formation is driven by strain energy minimization and demonstrates the periodicity of the misfit array that is in good agreement with experimental data using cross section high-resolution transmission electron micrograph (HR-TEM) images and also with other theoretical values.

Keywords: A1. Periodic interfacial misfit dislocations (IMF); A1. 90° misfit arrays; A3. Molecular beam epitaxy; B1. Alsb; B1. GaAs; B1. GaSb; B1. Si; B2. Semiconducting III–V materials

1. Introduction

The epitaxial growth of highly mismatched materials has been an important technological field for two decades. In particular, lattice-mismatched epitaxy of Sb-based materials on GaAs and Si substrates are attractive for advanced optoelectronic devices including monolithically integrated lasers [1,2], detectors [3,4], solar cells [5,6] and transistors [7,8]. Two prominent approaches to mismatched epitaxy involve either thick monolithic buffer layers or interfacial misfit dislocation (IMF) arrays [9–23]. The former growth technique involves tetragonal distortion within a critical thickness followed by misfit dislocation and often threading dislocations to alleviate strain in the bulk material [24]. Researchers often mitigate the deleterious effects by bending the vertically propagating defects along strained interfaces using compositionally graded-layers or selective area growth [25,26].

The latter approach involving IMF formation appears fundamentally different from the metamorphic approach as strain energy is immediately relieved at the interface by laterally propagating (90°) misfit dislocations confined to the epi-substrate interface [9–23]. After IMF array formation, subsequent material deposition proceeds in a strain-free layer-by-layer growth mode. Our experimental observations from cross-sectional high-resolution transmission electron micrograph (HR-TEM) images suggest that the IMF arrays exist along 110 and $1\bar{1}0$ directions in GaSb/GaAs [15] and AlSb/Si [22] systems. The goal of this paper is to describe these observations mathematically and to provide a detailed analysis of the periodic strain distribution in the IMF layer. Experimental data from Trampert et al. [11] is used as a reference for modeling InAs/GaAs system.

The IMF arrays can be formed using different growth techniques, such as, MOCVD [9,10], MBE [11–16],

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atmospheric pressure MOVPE [17] and wafer bonding [18]. The IMF arrays have been reported in several systems including GaP/Si [9], GaAs/Si [10], InAs/GaAs [11], InAs/GaP [12], GaSb/GaAs [14–18], InP/GaAs [21] and AlSb/Si [22,23] over a range of lattice-mismatched conditions ranging from $\Delta a_o/a_o = 0.4\%$ (GaP/Si) to $\Delta a_o/a_o \sim 13\%$ (AlSb/Si). To date, the IMF formation process has not been well established in the literature. Some researchers explain, on the basis of Matthews's theory that the IMF arrays form to relieve strain energy when the critical thickness is less than a single monolayer [24]. At first glance, this explanation seems logical for highly mismatched systems where $\Delta a_o/a_o > 10\%$ (AlSb/Si), but is not valid for low mismatch systems, such as GaP/Si ($\Delta a_o/a_o \sim 0.4\%$), in which the critical thickness is several hundred nanometers. Even in low mismatch systems, the IMF arrays relieve ~100% strain at the epi-substrate interface (i.e., before the critical thickness has been deposited).

2. Modeling IMF arrays

There are two equilibrium models describing critical thickness of lattice-mismatched systems. The first model by Van Der Merwe compares the energy of the composite system before and after the misfits are generated. The second model by Matthews considers forces acting on a dislocation to determine critical thickness. The concept of periodic IMF arrays was first introduced by Matthews and Blakeslee [24], which states that mismatched growth undergoes tetragonal distortion up to a critical layer thickness, beyond which it forms an array of misfit dislocations. This critical layer thickness, however, can only be calculated for low to moderate mismatch materials, $\Delta a_0/a_0 < 7\%$ and does not account for immediate IMF formation at a heteroepitaxial interface. However, Matthews's theory can be used to calculate the misfit spacing of IMF arrays as shown in Table 3. Frank and Van Der Merwe (FvdM) proposed a model based on the Frenkel and Kontorowa (FK) approach of truncated Fourier series [19] to describe the IMF formation mechanics. While based on a mechanical energy minimization principle, FvdM describes the atomic position and uniformly distributed strain energy within the framework of an entire bulk material system. Both these models assume pseudomorphic growth up to critical thickness. Thus, these models are not useful as a means for understanding periodic strain distribution at the interface where there is no pseudomorphic growth.

Kuronen et al. [20] introduced molecular mechanics (MM) to study the lattice-mismatched systems characterized by gliding dislocations, such as 30° and 60° misfits. The lattice is treated as a collection of weights connected with springs, where the weights represent the nuclei and the springs represent the bonds. Strain energy is calculated by summing the individual distorted bond energies derived using the stretch and bend equations described below. This approach is unique compared to the models described above [19,24] because it enables the calculation of strain energy based on individual atomic bonds. In the work done by Kuronen et al., strain is the driving force for 30° and 60° misfit formation and 90° dislocations are formed via conventional approach, that is by the interaction of two 60° misfits. In contrast, we observe an array of spontaneous 90° misfits that form at a heterointerface. Because of the nature of this IMF array formation it is not possible to use Kuronen's model to estimate strain in IMF arrays.

To describe the HR-TEM image results mathematically and to provide a detailed analysis of the periodic strain distribution in the IMF layer, an atomistic model, which considers atom–atom interaction and bond-energetics, is necessary. In this paper, we present a model based on MM to elucidate the strain energy distribution as a function of lattice site across the array. Our findings suggest that the IMF formation is driven by strain energy minimization. We focus on the GaSb/GaAs material system to compare and validate our theoretical results.

3. IMF arrays in GaSb on GaAs

Under specific growth conditions, GaSb deposited on GaAs (0 0 1) produces periodic 90° IMF arrays along both [1 1 0] and [1 $\bar{1}$ 0] [15]. The formation of 90° dislocations needs lowest elastic energy because of its large spacing compared to 60° misfits [18]. For that reason, 90° dislocations are energetically favorable in (0 0 1) semiconductor heterointerface compared to 60° dislocations, if the formation of 90° dislocations is unobstructed [18]. In our growth process, by observing the reflection high-energy electron diffraction (RHEED) pattern, we make sure that the formation of 90° dislocations is unobstructed as mentioned in our previous work [15]. The formation of 90° rather than 60° misfits requires balancing strain energy with adatom migration based on lattice mismatch, Sb overpressure and growth temperature for GaSb/GaAs system. Specific IMF formation conditions are discussed elsewhere [15].

Figs. 1(a) and (b) shows the GaSb/GaAs IMF array in a HR-TEM image and corresponding schematic illustrating atomic arrangement and bonding in the 100 plane around the interfacial misfit. The IMF appears as two bright spots in contrast to surrounding material to indicate strain. The HR-TEM micrograph of GaSb/GaAs sample is imaged under the bright field condition using multiple beams. Other TEM images related to GaSb/GaAs IMF array also exist in one of our publications [15], where the periodicity of the IMF array can be seen on a wide range. The bonds appear homogeneous and undistorted between misfits. The HR-TEM image provides resolution of individual lattice sites. Careful observation of the lattice shows that the misfit occurs every 14 Ga lattice sites, which is equivalent to 13 Sb lattice sites. The zinc-blende atomic arrangement seems undistorted in regions between the misfits.

We note that the ratio of lattice constants, a_f:a_s is equal to the ratio of IMF periodicity, x_s:x_f, where a_f, a_s are the