InAs Wires on InP (001)

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Abstract: The heterostructure of InAs/$In_{0.52}Al_{0.48}As$/InP is unique in that InAs wires instead of dots self-assemble in molecular beam epitaxy. These InAs wires have some distinctive features in their growth and structure. This paper summarizes the investigations of the growth and structural properties of InAs wires that have been performed in our laboratory recently.

Key words: quantum wires; InAs; MBE
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1 Introduction

Semiconductor quantum-confinement structures such as quantum wires (QWRs) and quantum dots (QDs) are of interest in both fundamental research and technological applications. Due to their distinctive one dimensional geometry, QWRs are less energetically favorable than QDs in mismatch heteroepitaxy. Therefore, they have been much less reported in the literature than self-assembled QDs. However, several reports have been made in recent years on the formation of InAs quantum wires on the InP (001) substrate by MBE[1~8]. Due to their distinct features in both geometry and energetics, the investigation of the growth and structural properties of InAs QWRs on InP (001) may help us to understand more about the self-assembling of semiconductor nanostructures using MBE. We present in this paper the studies performed recently in our laboratory on the growth and structural properties of InAs wires on InP substrate.

2 Growth of InAs wires on InP (001)

The samples were grown in both Gen-II and Riber 32-P MBE systems monitored in situ by reflection high-energy electron diffraction (RHEED). The buffer layer consisted of 300nm $In_{0.52}Al_{0.48}As$ on the InP (001) substrate. The mismatch between the buffer layer and the InP (001) substrate was determined by double crystal X-ray rocking curve to be less than 1.5×10^{-3}. InAs layers were deposited with a 3% mismatch on the $In_{0.52}Al_{0.48}As$/InP buffer at 500 ℃ by both the conventional MBE method and the MEE method[9]. For the MBE growth, the shutters of In and As cells were opened simultaneously, and the deposition rate was 0.1ML (monolayer)/s. For the MEE growth, the In and As shutters were opened alternately and the deposition rate was one atomic layer per second for In; the As shutter was opened for 2s in each cycle, and there was an interruption of 1s between the In and As pulses. The critical thickness for the 2D-3D transition is about 2.5ML of InAs deposition, as evidenced by the streaky-spotty transformation in the RHEED pattern.

3 Structural properties of self-assembled InAs QWRs on InP (001)

3.1 Self-assembled wires on InP (001) substrate

Figure 1 shows the transmission electron microscope (TEM) images. Figures 1(a) and (b) are the cross-section (002) dark-field images of the InAs wires in the six-stack InAs(7ML)/$In_{0.52}Al_{0.48}$-

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As(15nm) multilayer on the InP($\bar{0}$01) substrates. Figure 1(a), viewed along the [1$\bar{1}$0] direction, shows a cross-section of InAs wires, and Figure 1(b), viewed along the [110] direction, is the side view of them. These wires in the multilayer structure are stacked diagonally in the (001) growth direction, in contrast to the vertical alignment of InAs quantum dots on the GaAs (001) substrate. Figures 1(c) and (d) are plane-views of the InAs wires with diffraction vectors g = [110] and g = [$\bar{1}$10], respectively. With g = [$\bar{1}$10], parallel to the InAs wires, as shown in Fig. 1(d), the wire-like contrast disappears. The disappearance of the wire-like contrast in the TEM plane-view image with g = [$\bar{1}$10] demonstrates that the strain relaxation of the wires is one-dimensional along the [110] direction according to the criterion g · b = 0. The one-dimensional strain relaxation, normal to the wires, is consistent with the geometry of the quantum wires.

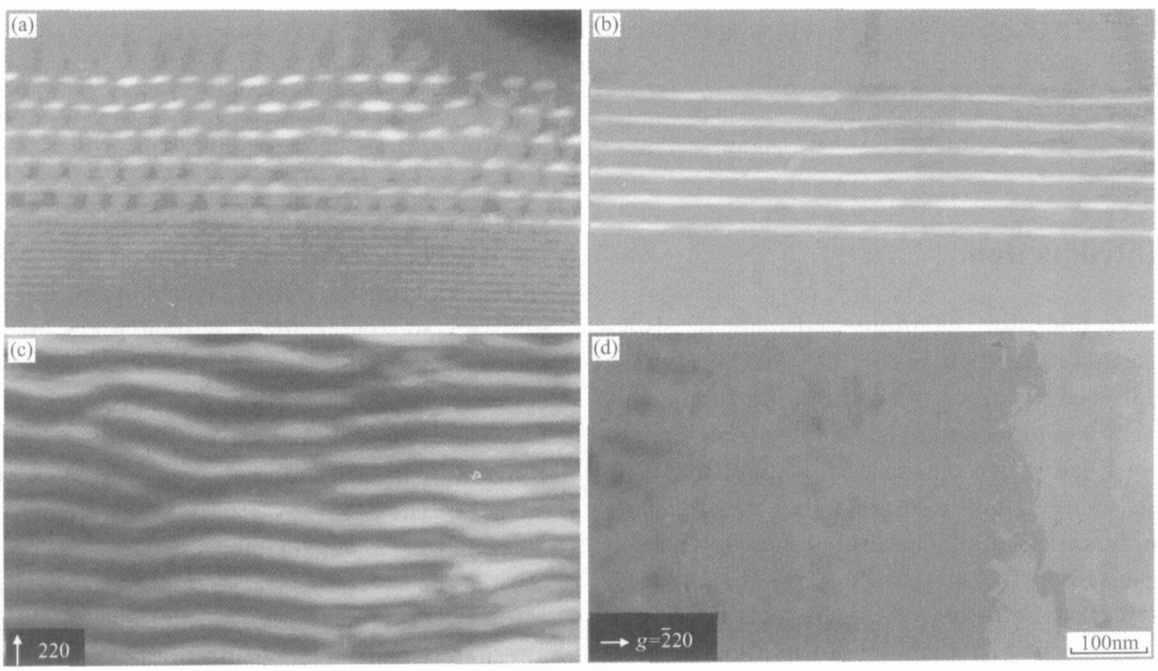

Fig. 1 TEM images of InAs wires (a), (b) Cross-section, (002) dark field, MBE, InAs(8ML)/$In_{0.52}Al_{0.48}As$(15nm), viewed along [110] and [$\bar{1}$10], respectively; (c), (d) Plane-view with g = [110] and [$\bar{1}$10], respectively

The driving force for the self-assembly of quantum dots or wires in a mismatch heterostructure is the volume elastic relaxation energy. For QDs, the mismatch strain undergoes relaxation in all directions, while for QWRs the component of the strain field in the direction along the wires remains equal to the value $\varepsilon_0 = (a_0 - a_s)/a_s$ throughout the entire wire, where a_0 and a_s are the lattice constants of the epilayer and the substrate, respectively. Therefore, the volume elastic relaxation is more efficient for QDs than for QWRs. A comparison of the quantum dots and the quantum wires in energetics indicates that the mechanism for the formation of wires instead of dots is related to kinetics rather than energetics.

3.2 Calculation of the strain distribution of the InAs wires

It is well known that quantum dots in a multilayer InAs/GaAs (001) system are vertically stacked along the [001] growth direction. This vertical alignment is caused by the partial strain relaxation in the GaAs spacer layer. The partial strain relaxation is maximal just above the quantum dots, and the nucleation and growth of quantum dots in the next layer are much more probable on the top of the quantum dots in the layer below. However, the arrangement of the InAs wires in the InAs/InAlAs multilayer structure is quite distinctive in that they are stacked diagonally a-

long the growth direction, as shown in Fig. 1. Such a distinction of InAs wires in alignment implies that the strain distribution in the InAlAs spacer layer induced by an InAs wire is significantly different from that of the InAs dots in GaAs.

As mentioned in the last section, the strain relaxation of the wires is perpendicular to the wires and is totally restrained in the direction along the wire. Therefore, the strain distribution of the wires is two-dimensional and is much more easily analyzed than that the strain distribution around a dot by both numerical calculation and analytic methods. We perform the numerical calculation of the strain distribution around a wire using the finite element method[2], and the results are consistent with experimental observations.

It has been clarified by X-ray analysis that the strain field inside or nearby a quantum wire in a heteroepitaxy mismatch system is highly inhomogeneous[10,11], which indicates that these wires cannot be treated with a simplified strain model. However, in this work, we are only concerned with the far-reaching elastic distortion induced by the presence of the wires in the matrix rather than the strain distribution inside or nearby the wires. From the cross-section of the wire shown in Fig. 1, it can be seen that the width-to-height ratio is as large as 4～5, and its effect may be similar to that produced by a strained ribbon in far regions in the matrix. Therefore, in our calculation, the wire section is approximated by a line segment of original length L_0 in an isotropic two-dimensional matrix of indefinite dimension, as shown in Fig. 2. The line segment is homogeneously stretched lengthwise by 3%, which is equal to the mismatch between the InAs and the $In_{0.52}Al_{0.48}As$ matrix, and the region surrounding it is elastically distorted to some extent. The angular distribution of the elastic distortion above the strained line segment is calculated with the finite element method. In the calculation, Poisson's ratio and Young's modulus are taken to be 0.36 and 6.07×10^{10} Pa, respectively, similar to those in InP[12]. Figures 3(a) and (b) show the calculated components ε_{xx} and ε_{yy} of the elastic strain field around the line segment with the 3% elastic extension in the matrix. The figures show that the maximum elastic distortion is not above the wire but staggers away, and the strain angular distribution is skewed away from the wire's top. Although the calculation is performed for the matrix with infinite dimension, the results may be appropriate to the practical situation if the influences of the boundary and the interaction between the extended segments are not significant. During the epitaxial growth of the strained InAs film on the InAlAs spacer layer, the quantum wires will nucleate and grow in the region where the values of the components of the elastic strain field are the maximum. As calculated, the strain maximum in each InAs layer is arranged in a staggered pattern, as experimentally observed, the InAs wires are diagonally arranged in the multilayer structure. Therefore, the calculation is consistent with experimental observation.

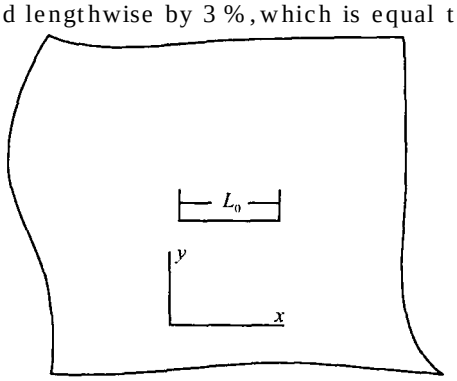

Fig. 2 Strain model for InAs wire in the $In_{0.52}Al_{0.48}As$ matrix

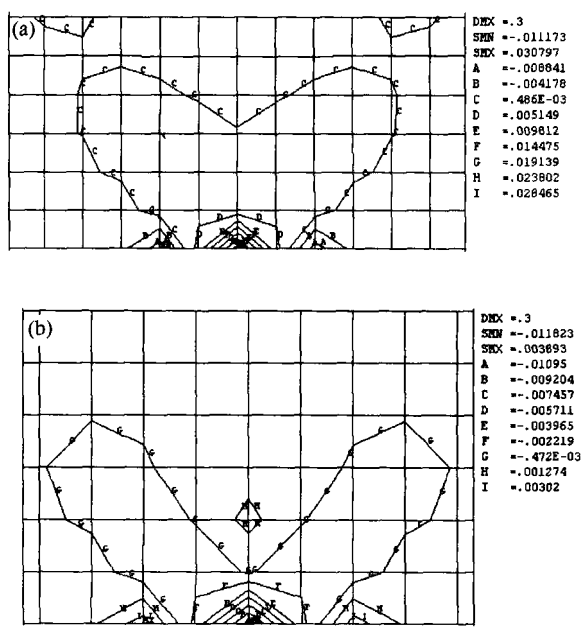

Fig. 3 Angular strain distribution around an InAs wire in the $In_{0.52}Al_{0.48}As$ matrix as calculated using the finite element method

3.3 Influence of spacer composition on InAs wire arrangement

It was found that the composition of the matrix has some significant influence on the arrangement of the InAs wires in a multilayer structure[3]. When the spacer is a $(In_{0.52}Al_{0.48}As)_m/(In_{0.53}Ga_{0.47}As)_n$ short-period superlattice (SPSL) instead of $In_{0.52}Al_{0.48}As$, where the integers m and n are the numbers of the respective monolayers, the diagonal arrangement of the InAs wires transforms to a vertical one in which n increases relatively to m. Figures 4(a) and (b) are TEM images of the InAs wire arrays in the $(In_{0.52}Al_{0.48}As)_4/(In_{0.53}Ga_{0.47}As)_2$ matrix and in the $(In_{0.52}Al_{0.48}As)_2/(In_{0.53}Ga_{0.47}As)_2$ matrix, respectively. The figures demonstrate that the InAs wire arrangement is transformed from diagonal to vertical as the ratio m/n is reduced from 4/2 to 2/2. Such a transformation in wire arrangement cannot be interpreted with the simple model proposed in the last section. To understand the exact mechanism requires more experimental investigation.

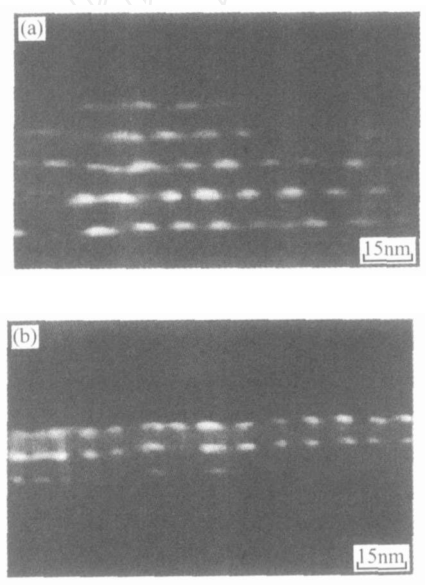

Fig. 4 Cross-section TEM images of InAs wires, (002) dark field (a) InAs(8ML) in $(In_{0.52}Al_{0.48}As)_4/(In_{0.53}Al_{0.47}As)_2$; (b) InAs(8ML) in $(In_{0.52}Al_{0.48}As)_2/(In_{0.53}Al_{0.47}As)_2$

3.4 Influence of growth mode on the symmetry of wire arrangement

3.4.1 Symmetry in InAs wire alignment

In our investigation of InAs/InP nanostructures, the InAs is deposited with both the MBE and the MEE method. The distinction between the two epitaxial modes is that for the MBE mode, the group Ⅲ and Ⅴ elements are deposited simultaneously on the growth surface, while for the MEE mode the group Ⅲ element and the group Ⅴ element are deposited in succession to enhance the migration of the group Ⅲ adatoms on the growth surface. Such an enhancement in migration is generally believed to improve the morphology of the flat epitaxial film.

The growth mode has some influence on the structural properties of the wire array in the InAs/InAlAs/InP(001) system[4]. Figure 5 shows cross-sectional TEM images of the InAs wire array viewed from the [1$\bar{1}$0] direction. Figure 5(a) is the MBE InAs/$In_{0.52}Al_{0.48}As$ wire array on the InP(001) substrate, the InAs thickness is 8ML. The InAs wires in the array are stacked along directions about 33° away from the [001] growth direction on either side, and the wire array is symmetrical about the [001] growth direction. Such symmetry in the MBE wire array on InP(001) is disrupted when the epilayer is grown on the substrate disoriented from (001) or grown with the MEE mode. Figure 5(b) is the asymmetrical MBE InAs wire array on the InP substrate 6° misoriented from (001) towards the (111) Ga plane, and the angles between the growth direction and wire alignment are 26° and 43°, respectively, on the two sides in the figure. Figure 5(c) is the asymmetrical MEE InAs(8ML)/$In_{0.52}Al_{0.48}As$(15nm) wire array on the InP(001) substrate, and the angles between (001) and the wire alignment are 47° and 38°, respectively, on the two sides. Figure 5(d) is the asymmetrical MEE InAs(10ML)/$In_{0.52}Al_{0.48}As$(15nm) wire array, and the slanting angles are 30° and 70°, respectively. Obviously, as the thickness of InAs is increased from 8ML to 10ML, the asymmetry in the MEE InAs wire alignment increases. In addition, the QWR cross-section shape in the figure is apparently distorted from a symmetrical one about the [001] growth direction.

3.4.2 Discussion of the symmetry of the InAs wire alignment

The [001] direction is symmetrical in crystallography and it is easy to understand that the MBE-InAs-wire array on the InP(001) substrate is

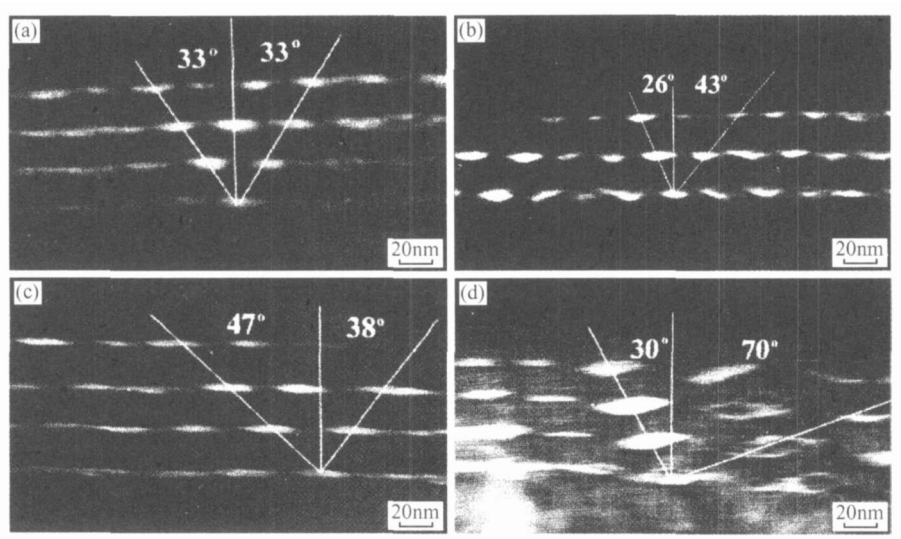

Fig. 5 Cross-section TEM images of InAs wires, (002) dark field (a) MBE, InAs(8ML)/$In_{0.52}Al_{0.48}As$(15nm) on InP(001); (b) MBE, InAs(8ML)/$In_{0.52}Al_{0.48}As$(15nm) on misoriented InP(001); (c) MEE, InAs(8ML)/$In_{0.52}Al_{0.48}As$(15nm); (d) MEE, InAs(10ML)/$In_{0.52}Al_{0.48}As$(15nm)

symmetrical about the growth direction and that the symmetry is disrupted when the material is grown on the disoriented (001) substrate. However, the asymmetry in the alignment of the MEE InAs wire array on the exact (001) substrate is worthy of some discussion.

The main difference between the MBE and the MEE growth modes is that the surface atomic diffusion during growth is significantly enhanced in the MEE mode relative to that in the MBE mode[9]. The asymmetry in the MEE InAs wire array may be related to the enhanced diffusion kinetics, and the mechanism we proposed is as follows.

Figure 6 is a schematic cross section of an InAs wire under self-assembly during MBE epitaxial growth. The hills at both sides A and B in the figure are built up with terraces and steps in atomic scale. Uphill migration of adatoms randomly deposited on the growth surface is necessary for the wire to self-assemble and the driving force for adatoms' ascending motion is strain energy, as an In atom incorporated on a top site would be in a more relaxed strain state. If the terraces and steps on sides A and B are different from each other in the atomic structure, the energy barriers for the ascending adatoms are different, and the upwards motion is biased with more adatoms migrating uphill from the side with the smaller energy barrier. This biased uphill motion of adatoms may result in the asymmetry in the MEE InAs wire array on the exactly (001) oriented substrate.

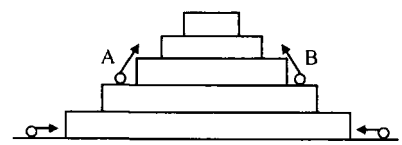

Fig. 6 Schematic representation of an InAs wire under self-assembly

Indeed, the steps on hills A and B are different from each other in atomic structure. Figure 7 is a structural model of the (2×4) GaAs(001) reconstructed surface in the α-phase[13]. The strained InAs film on the GaAs(001) is also (2×2) reconstructed[14] and may be similar to the (2×4) GaAs (001) reconstructed surface in atomic structure. A long terrace of one ML height along the $[\bar{1}10]$ direction should be formed with complete (2×4) units to keep the charge neutral. Therefore, the two edges of a terrace should be different from each other in atomic structure due to surface reconstruction, resulting in different energy barriers for atoms ascending up hills A and B. With more adatoms ascending up the hill from the side with the lower energy barrier, the symmetry of the wire cross section would be distorted and the resulting angular distribution of the mismatch strain would not be symmetrical about the growth direction. Eventually, the asymmetrical strain distribution produces an asymmetry in the InAs wire array on the (001) substrate, as experimentally observed in

this work.

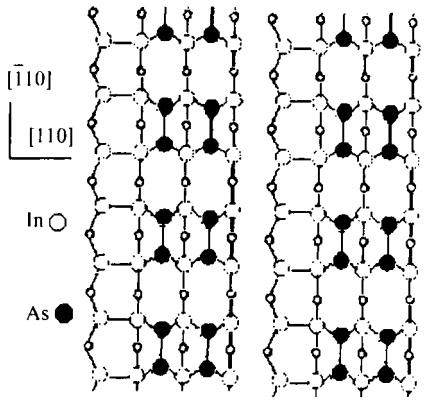

Fig. 7 Schematic GaAs (2 ×4) reconstructed surface

For the MBE growth mode, the atomic diffusion is reduced in comparison with the MEE mode and the effect proposed above may be neglected, and the MBE InAs wire array seems symmetrical about the [001] growth direction.

4 Summary

As summarized above, InAs wires in a InAs/ $In_{0.52}Al_{0.48}As$/ InP system are somewhat distinctive in structure: they are diagonally aligned along the growth direction, and the symmetry in the vertical wire arrangement is associated with the MBE growth mode. Investigation of these specific properties of InAs wires may help us to understand more about the self-assembly of nanostructures in semiconductor heteroepitaxy.

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InP(001)衬底上的 InAs 量子线

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摘要：在分子束外延生长的 InAs/$In_{0.52}Al_{0.48}As$/InP 异质结体系中，形成 InAs 量子线. 这些 InAs 量子线在生长和结构方面有一些独到的特性，并介绍了本实验室在研究 InAs 量子线的生长和结构方面所做的工作.

关键词：量子线；InAs；分子束外延

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