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## Plastic Relaxation Mechanics in Systems with a Twist-Bonded Layer

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### ABSTRACT

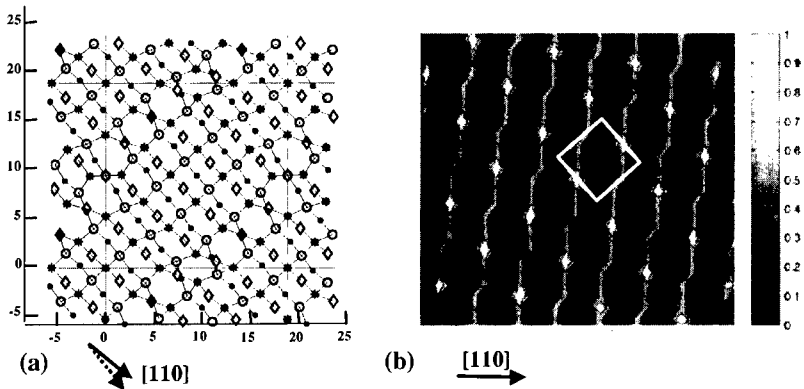
With a view to investigating how a thin film twist-bonded to a host substrate can have compliant behavior from a plasticity point of view, the onset and spread of edge dislocations throughout a mesa are studied. The discussion focuses on the energy relaxed by such dislocations in a mesa made from two coherently bonded lattice-mismatched layers twist-bonded onto a host substrate and patterned down to the film/host substrate interface. Our theoretical results show that the confinement of threading dislocations into a thin twist-bonded film is energetically favorable allowing the overgrowth of a mismatched layer exempt of any threading dislocation at least as far as mesas are concerned.

### INTRODUCTION

Manufacturing high-performance optoelectronic devices requires the growth of semiconductor heterostructures exempt of any defects, especially those that result from stress relaxation. Actually, such manufacture is inhibited by the lack of appropriate substrates allowing the growth of highly lattice-mismatched heterostructures. Indeed, when a film is grown lattice-mismatched on a substrate by techniques like MBE (Molecular Beam Epitaxy), its stress energy increases with thickness up to a critical point beyond which it has to be released by either an elastic (formation of dots) or a plastic (formation of dislocations) process. Therefore, engineering a somewhat "universal" substrate, i.e., "compliant" with any kind of epitaxial growth is currently one of the most challenging goals in materials research for optoelectronics [1-5]. In 1991, Lo [1] initiated the subject by suggesting the use of a thin film as substrate. As a matter of fact, the law ruling the way the elastic energy is shared by the two films means the thicker will impose its own lattice parameter onto the thinner, which will therefore sustain most of the defects arising from stress relaxation. The next problem to be solved is the unavoidable curvature and the difficult mechanical handling of such an ultra thin heterostructure. Several solutions have already been proposed to tackle this problem, most of them involve sticking the compliant substrate on a thick host substrate. The way this sticking is done reveals the way the relaxation is presumed to act. If an intermediate viscous layer is used to stick the compliant layer to its host substrate, an elastic relaxation is guessed acting [6,7] whereas any attempt to weaken the interface by for example twisting and/or tilting the compliant axes relative to the host substrate ones means that some kind of plastic relaxation is expected [8-13].

In this study, we concentrate on the plastic relaxation undergone by a heterostructure made of two lattice-mismatched layers, twist-bonded to a host substrate. At this point, it is worth noting that when dealing with the concept of compliance, the film cannot be considered as laterally infinite but must be regarded as a finite mesa because edges are the most favourable places for a dislocation to initiate or end. This paper is the second one dedicated to the subject. In

the first one [14], we made use of a Keating formalism to describe the chemical bonding at the twist-bonded interface for twist angles smaller than  $16^\circ$ . As far as rectilinear edge dislocations are concerned, their energetically best locations have been proved to be at the heterointerface and not at the twist-bonded interface. Besides, we have proposed a new type of dislocations called “kinked edge dislocations” shaped to better fit the twist-bonded interface features than rectilinear edge dislocations do. Both rectilinear edge dislocations and kinked edge dislocations have to face a significant energy barrier when penetrating from a mesa edge towards the mesa center, either at the heterointerface or at the twisted interface. In the present paper, we will continue this study with special attention paid to the role played by the threading dislocations on the edge dislocation spreading into the sample, the latter being among the most damaging defects for optoelectronics applications.

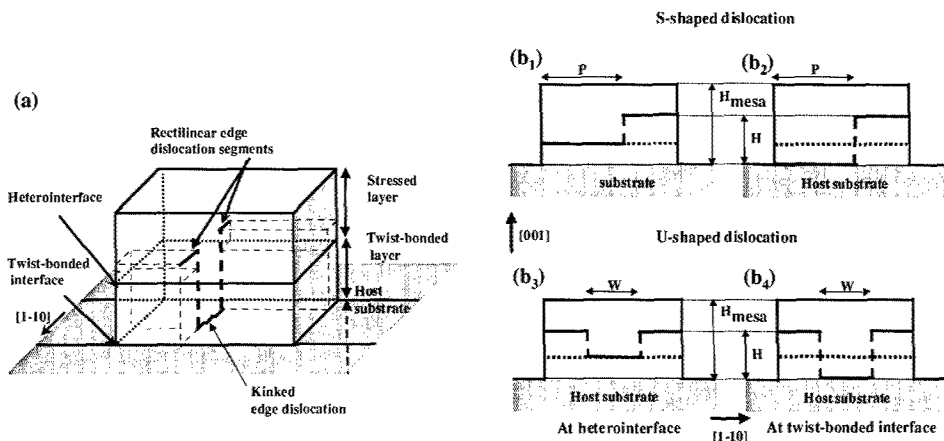


**Figure 1. a)** The  $\Sigma_{25}$  ( $\theta=16.26^\circ$ ) twist-bonded interface: P- and In-atoms are tagged by circles and points in the host substrate, by star and square in the twist-bonded layer, respectively. The  $sp^3$  bonds are marked by lines. Dashed and solid arrows indicate the  $[110]$  direction for the host substrate and the twist bonded layer, respectively. **b)** Energy map for the  $\Sigma_{25}$  ( $\theta=16.26^\circ$ ) twist-bonded interface. The white square indicates the  $\Sigma_{25}$  period boundaries

# METHODOLOGY

To study compliance effects a model structure is constructed out of a heterostructure made of two (001) zinc-blende mismatched layers twist-bonded to a (001) host substrate. The whole structure is made of material having the same InP stretching force constants but the uppermost layer is stressed by assuming a lattice parameter 4% greater than that of the other two. The thickness is 32 atomic layers for the stressed layer (thus beyond the usual plastic critical thickness) but only 8 atomic layers for the twist bonded layer (thus below the usual plastic critical thickness). The system displays two interfaces along the  $[001]$  axis: i) a heterointerface between the lattice-mismatched layer and the twist-bonded layer and ii) a twist-bonded interface between this twist-bonded layer and the host substrate below. The position of rows of atoms above (below) the twist-bonded interface is denoted by integer numbers  $n_1$  and  $n_2$  ( $n_3$  and  $n_4$ ) in surface lattice units along the  $[110]$  and  $[1-10]$  directions. The twist-bonded layer and the host substrate

are rotated one with respect to the other around the  $[001]$  axis by  $16.26^\circ$  that corresponds to the grain boundary  $\Sigma_{25}$ . The relaxed  $\Sigma_{25}$  atomic positions in the twist-bonded interface and the corresponding map energy are shown in Figure 1. This interface is stabilized, assuming that no dangling bonds remain. Afterwards, a 100-atomic-row wide square mesa is designed by patterning the so-defined heterostructure down to the twist-bonded interface as shown in Figure 2a.



**Figure 2.** a) Schematic diagram of a mesa formed from a heteroepitaxial film deposited on a twist-bonded substrate on a thick host substrate. b) Diagram showing S-shaped dislocations and U-shaped dislocations bottomed either at the heterointerface or at the twist-bonded interface. The bottom segment is either rectilinear at the heterointerface or kinked at the twist-bonded interface.

The next step in our theoretical approach addresses the way threading dislocations could be confined in a twist-bonded layer. We define in Figure 2b two kinds of dislocations, namely, the “S-shaped” and the “U-shaped” dislocations. As can be seen in Figure 2b, “S-shaped” dislocations consist of an edge (rectilinear) dislocation segment located on the twist-bonded interface (heterointerface), starting at a mesa edge, penetrating into the mesa up to depth  $P$  and ended by a threading dislocation gliding up to height  $H$  towards the surface. Another rectilinear edge dislocation segment starts from this threading dislocation extremity, goes and reaches the other mesa edge. Indeed, the strong interaction between close dislocations forbids the return to the same mesa edge. Note that some “S-shaped” dislocations have a special pattern: i) a threading dislocation ending at a height  $H$  equal to the mesa height ( $H_{\text{mesa}} = 40$  atomic rows) signifies a threading dislocation emerging at the mesa surface and thus a pattern devoid of a second edge dislocation segment. These special S-shaped dislocations will be named “L-shaped” in the following, ii) a null penetration depth  $P$  corresponds to a system without any kind of edge (for  $H = H_{\text{mesa}}$ ) or threading dislocations (for  $H < H_{\text{mesa}}$ ), iii) a penetration depth  $P$  equal to the mesa width (100 atomic rows) means an edge dislocation heading straight through the whole mesa and thus a system with no threading dislocations. Let us consider now “U-shaped” dislocations they involve an edge dislocation segment (width  $W$ ) also lying on the twist-bonded interface but now set

symmetrically relative to the mesa middle. Therefore, two threading dislocations emerge one at each of the segment ends and travel through the mesa toward the surface up to height  $H$ . The pattern is completed by two edge dislocation segments placed on both sides of the initial segment and finishing at the opposite mesa edges for the same reason as above. Here again, there are some special cases of interest: i) if width  $W$  is zero, the pattern contains no dislocation at all, ii) if the segment width is equal to the mesa width, there is just a single transverse edge dislocation, and finally iii) if height  $H$  is equal to the mesa height, the system includes two surface-ended threading dislocations enabling us to give an estimation of a threading dislocation cost. The bottom segment is always of the kinked type if at the twist-bonded interface, but of the rectilinear kind elsewhere.

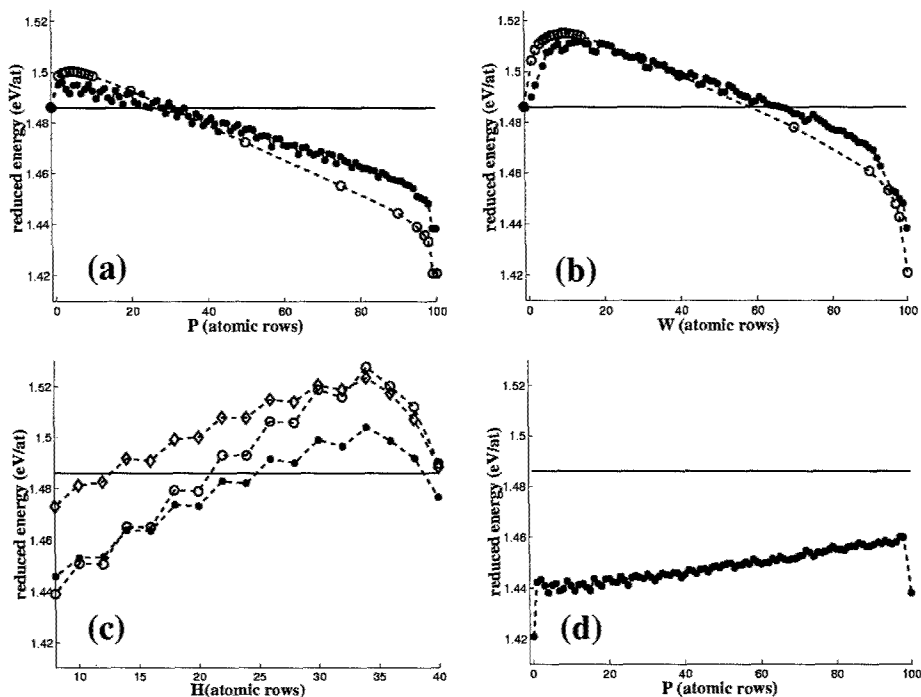
## RESULTS AND DISCUSSION

Figure 3 displays the reduced energy (energy normalized by the average atom number contained in a mesa plane) for various kinds of dislocations making their way into the mesa along the  $[1\ -1\ 0]$  direction. In Figure 3a, the curve marked by circles shows the reduced energy variation versus the penetration depth  $P$  for an L-shaped rectilinear edge dislocation located at the heterointerface (schematized in Fig 2b<sub>1</sub>, with  $H=H_{\text{mesa}}$ ). A simple look at this curve indicates that the dislocation faces a 30-atomic-row wide and 15meV-high energy barrier to break into the mesa. Actually, this barrier energy is thought to be small enough to be overcome especially in a growth process. If so, the more the dislocation progresses into the mesa the more the mesa elastic energy will be released. In the same Figure 3a, the curve labeled by points deals with an L-shaped dislocation with a bottom kinked edge segment at the twist-bonded interface (schematized in Fig 2b<sub>2</sub>, with  $H=H_{\text{mesa}}$ ). The periodic oscillations shown by this curve result from the crossing by the dislocation of regularly spaced strongly (light gray in Fig.1b) and weakly (dark gray in Fig.1b) stressed regions according to  $\Sigma_{25}$  periodicity. This oscillating behavior allows the original energy barrier to be split into a succession of lower (few meV) and narrower (4 atomic rows) ones and thus makes it easier to pass through via a step-by-step process. However, note that the ensuing progression enables less energy to be released than in the previous case for penetration depths greater than 25 atomic rows.

Let us turn now to the hypothesis of a dislocation nucleation in the mesa core itself. Figure 3b presents reduced energy curves versus dislocation width for mesa-centered U-shaped dislocations with a bottom rectilinear segment at the heterointerface (circles) or a bottom kinked segment at the twist-bonded interface (points) schematized in Fig.2b<sub>3</sub> or Fig.2b<sub>4</sub>, respectively. In both cases, the associated threading dislocations end at the surface. When comparing Figure 3b with Figure 3a, it is clear that the curves are on the whole shifted towards higher energy because of the cost in energy required by two threading dislocations now instead of only one as previously. Second, in both cases, the energy decreases as the U-dislocation bottom widens, that is to say, when the interaction between the threading dislocations diminishes as they move apart and the elastic strain is relaxed on a larger area. These two points clearly underline the key role played by threading dislocations in the total energy balance: their cost in energy in a nucleation process protects the system from any kind of dislocation nucleation inside a mesa when other relaxation processes such as introduction from edges are available.

In other respects, limiting the threading dislocation extension itself can also be of importance in terms of reduced energy. Figure 3c highlights this point by showing the reduced energy of an S-shaped dislocation for  $P=11$  atomic rows (circles) and  $P=45$  atomic rows (points) on the one hand, and on the other hand of 60-atomic-row wide U-shaped dislocation (diamonds) as a

function of their height  $H$ . The common trend of these three curves is that the energy decreases with height down to a minimum when threading dislocations are confined in the twist-bonded layer, viz, for  $H=8$  atomic rows. In Figure 3d, the variation of S-shaped dislocation topped with a rectilinear edge dislocation segment at the heterointerface and bottomed with a kinked edge dislocation segment at the twist-bonded interface (see Fig. 2b<sub>2</sub> with  $H=H_{\text{mesa}}$ ) is shown as a function of the penetration depth  $P$ , i.e. the lateral position of the threading dislocation into the twist-bonded layer. As expected, the energy increases linearly as the kinked edge dislocation segment penetrates deeper and deeper into the twist-bonded interface, indicating by the way that the most suitable location for edge dislocation is at the heterointerface.



**Figure 3:** Reduced energy **a)** versus penetration depth  $P$  for an L-shaped dislocation located either at the heterointerface (circles) or at the twist bonded interface (points). **b)** versus width  $W$  for a U-shape dislocation located either at the heterointerface (circles) or at the twist bonded interface (points), the threading dislocations emerging at the surface ( $H=40$ ). **c)** versus height  $H$  for an S-shaped dislocation for  $P=11$  atomic rows (circles) and  $P=43$  atomic rows (points) and for U-shaped dislocation with  $W=60$  atomic rows (diamonds). **d)** versus threading dislocation location  $P$  (see text) for S-shaped dislocations with  $H=8$  atomic layers. The horizontal solid line indicates the reduced energy for a mesa without any dislocation.

## CONCLUDING REMARKS

In this paper, we have dealt with questions about plastic relaxation in a so-called compliant systems. For this, we have considered a mesa cut out of a heterostructure twist-bonded to a host substrate and we have focused on misfit dislocations in such a system. The latter displays two interfaces where misfit edge dislocation can originate, viz, a heterointerface and a twist-bonded interface. At both these locations, edge dislocations have to confront an energy barrier prior to moving ahead through the mesa. It appears that misfit dislocations located at this twist-bonded interface enter in an easier way from the edge of the sample than those located at the heterointerface. Actually not all edge dislocations totally cross through the sample and residual threading dislocations are usually present. Their cost in energy is the key point in compliance mechanisms. We have thus studied several different types of misfit dislocations, ended by threading dislocations, located either in the overlayer or in the twist-bonded layer. It turns out that the best design for releasing stress energy is an S-shaped dislocation fully confined within the twist-bonded layer. The unavoidable residual threading dislocations are thus kept away from the overlayer what is most important for technological applications.

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