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Rapid communication

Twist wafer bonded “fixed-film” versus “compliant” substrates: correlated misfit dislocation generation and contaminant gettering

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Abstract. *Compliant* film substrates, which ideally are free-standing thin-film substrates, can be used to grow lattice-mismatched hetero-epitaxial films without misfit dislocation generation to thicknesses beyond the usual critical conditions, because the elastic strain is shared by the epitaxial and the substrate films. Some recent studies have shown that hetero-epitaxial films of superior quality have been grown on thin substrate films fixed to bulky handle wafers obtained via the wafer-bonding method at a rotation angle, which produced a relaxed twist boundary consisting of a screw dislocation network. We consider it as highly unlikely that during growth of the hetero-epitaxial film such a fixed film can be elastically deformed to resemble a free-standing compliant thin-film substrate. In this rapid communication, a tentative interpretation of the role of the fixed-film substrate in producing high-quality hetero-epitaxial films is presented: (i) the screw dislocations gettered away contaminants that would otherwise lead to the generation of growth stacking faults; and (ii) the screw dislocations also allowed the misfit dislocations to be generated in a *correlated* way so that few threading dislocation segments were left in the bulk of the hetero-epitaxial film.

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For the fabrication of a wide variety of low-defect-density materials with different lattice constants for electronic and optoelectronic applications, the use of *compliant* substrates for growing epitaxial films has become a vigorously pursued subject. A hetero-epitaxial film (HEF) grown on a bulk substrate is initially pseudomorphic with the lattice mismatch accommodated elastically. The elastic strain is relaxed by the generation of misfit dislocations when the hetero-epitaxial film thickness exceeds a certain value, usually taken to be the Matthews–Blakeslee critical thickness [1, 2] obtained by energy balance considerations not including the dislocation nucleation kinetics. This relaxation process leaves many threading dislocation segments in the film. Ideally, a compliant substrate is a free-standing thin-film substrate so that initially the misfit can be accommodated by elastic deformation shared by the two films [3–6], leading to a strained hetero-epitaxial film of a larger useful thickness before relaxation occurs, at the price of film bending and handling difficulties. To overcome these problems, substrates consisting of a fixed film (FF) on a handle wafer (HW) have recently been used, leading to the growth of $In_{0.35}Ga_{0.65}P$ films with few defects [7], and to $In_{0.03}Ga_{0.97}As$ films with fewer defects and a larger elastic strain [8]. These FF–HW substrates, assumed to be still compliant elastically, are obtained by a wafer-bonding process: the ‘compliant’ layer is a [001] GaAs thin film, grown on a layer of AlAs which was grown on a sacrificial GaAs wafer first, welded face down to a [001] GaAs handle wafer via wafer bonding. The sacrificial GaAs wafer is then removed by chemical etching with AlAs acting as an etch-stop layer. Subsequently, the AlAs layer is etched away, exposing the bottom surface of the original ‘compliant’ film as the fixed-film top surface. The GaAs FF–HW boundary structure of Carter-Coman et al. [8] is not known, but it should be a low-angle boundary. That of Ejeckam et al. [7] is a relaxed twist boundary consisting of a screw dislocation network.

It is hard to believe that the GaAs fixed film [7, 8] can still be elastically compliant to a heteroepitaxial film, because this would require that the fixed film were displaced relative to the handle wafer on a macroscopic scale, which in turn requires the FF–HW boundary to slide on the GaAs (001) plane to the same scale, which can be facilitated only by grain boundary dislocations. Since dislocations in GaAs can only glide on {111} planes and not on {001} planes, and for the twist FF–HW boundaries the two perpendicular sets of intersecting screw dislocations must move apart, and hence will produce jogs and point defects, it is unlikely that the fixed film can easily slide on the handle wafer. Thus, the fixed film should be elastically noncompliant. Assuming this to be the case, we need to find other explanations for the role of these GaAs fixed films in producing hetero-epitaxial films with a superior quality. The purpose here is to suggest such an alternative explanation.

From the transmission electron micrographs obtained by Ejeckam et al. [7], it cannot yet be judged with certainty how much the density of threading dislocations was reduced in their $In_{0.35}Ga_{0.65}P$ heteroepitaxial film grown on a fixed film, but a major benefit due to gettering of contaminants by the screw dislocations at the FF–HW boundary is apparent. Some of the clearly visible defects in the TEM micrograph of an hetero-epitaxial film grown on a bulk GaAs substrate appear to be growth stacking faults typical of those of an epitaxial film grown on a contaminated substrate, e.g., those in epitaxial Si grown on Si wafers at high temperatures using a worn-out Si_3N_4-coated graphite susceptor, which released carbon to contaminate the Si substrate surface. The In-containing heteroepitaxial film used by these authors were grown via either the MOCVD method [7] or the MBE method [8], for which carbon is a common contaminant. Thus, it is not surprising that hetero-epitaxial films grown on GaAs bulk substrates contain many growth stacking faults. These defects are not present in the hetero-epitaxial film grown on the fixed film used by Ejeckam et al. [7], apparently because the screw dislocations have gettered the carbon contaminants away from the fixed-film surface, leaving it clean for the growth of a stacking-fault-free hetero-epitaxial film. Gettering of contaminants away from device-active regions in Si is an extensively investigated subject [9–11]. Since Si is an indirect-band-gap semiconductor, impurity atoms and defects control the Si bulk minority-carrier lifetimes and the reverse bias leakage currents at the Si pn junction. Presently, gettering is the prevailing technology, ensuring a high leakage-limited yield for manufacturing devices on bulk as well as epitaxial Si substrates. On the other hand, gettering is unexplored in compound semiconductors, because most materials have a direct band gap and hence the carrier lifetimes are not controlled by impurities and defects. It is important to note from the present discussion that gettering can improve the quality of the epitaxially grown compound materials.

It appears that gettering may be largely responsible for the results obtained by Carter-Coman et al. [8]. The misfit between their $In_{0.03}Ga_{0.97}As$ hetero-epitaxial film and the fixed film is small, $\sim 0.1\%$, indicating a large critical film thickness, ~ 1000 Å, which is also their fixed-film thickness. Their hetero-epitaxial film thicknesses range from 2000 to 8000 Å. Hetero-epitaxial film growth without the presence of a fixed film and gettering will relax at a thinner thickness than that for those on fixed-film substrates, because the stacking faults and carbon aggregates are low-energy sites for nucleating misfit dislocations, although they are not misfit relief defects per se. Without such low-energy sites in the hetero-epitaxial films on fixed-film substrates, relaxation does not need to occur in the strained layers exceeding the critical thickness by a few times. The misfit between the $In_{0.35}Ga_{0.65}P$ hetero-epitaxial film and the GaAs fixed film used by Ejeckam et al. [7] is large, $\sim 1\%$. This results in a fairly small critical film thickness, ~ 100 Å, which is also their fixed-film thickness. Their heteroepitaxial film grown to the thickness of 3000 Å, i.e., to ~ 30 times the critical thickness, is apparently defect free. Since gettering alone can hardly be responsible for this large difference, another mechanism should be also operational. We suggest a *correlated* misfit dislocation generation mechanism, discussed below.

We suggest that the $In_{0.35}Ga_{0.65}P$ hetero-epitaxial film of Ejeckam et al. [7] have been partially or fully relaxed by misfit dislocations. As induced by the presence of the screw dislocations at the FF–HW boundary, the misfit dislocation network at the HEF–FF interface is likely to be arranged in an orderly manner with few threading dislocation segments in the hetero-epitaxial film bulk. The suggested process leading to this situation may be termed a *correlated* misfit dislocation formation process. This relaxation process should have been started at a hetero-epitaxial film thickness thinner than that without the fixed film, because, provided the fixed film is elastically noncompliant, the film on the fixed film is higher in elastic energy. The hetero-epitaxial film without the fixed film has a dilatational strain in the plane of the film. At the same thickness, that on a fixed film has the same dilatational strain together with a shear strain inherited from the fixed film because of the FF–HW twist boundary.

There are two possible ways the $In_{0.35}Ga_{0.65}P$ hetero-epitaxial film on a fixed film studied by Ejekam et al. [7] could relax without leaving threading dislocations. First, the misfit dislocations may be nucleated from the FF–HW boundary screw dislocation nodes, which move across the fixed-film layer to reach the HEF–FF interface. In this way, any threading dislocation segments left are in the fixed-film layer instead of in the hetero-epitaxial film. This process deforms the fixed film plastically to make it conform to the hetero-epitaxial film lattice constant. Now, the film is a compliant substrate, but the mechanism is that of plastic deformation and not that of sharing the elastic strain as originally envisaged for the role of a compliant film substrate.

The second way is the nucleation of misfit dislocation half-loops from the weakly-bonded or high-energy positions on the hetero-epitaxial film surface, each of which can leave two threading dislocation segments in the hetero-epitaxial film bulk. In hetero-epitaxial films on normal substrates, the nucleation positions are *randomly* distributed, and hence these half-loops and threading dislocation segments are also randomly distributed. This means the probability that a pair of threading dislocation segments, one from a different half-loop, can annihilate each other is small. Thus, relaxed hetero-epitaxial films on bulk substrates usually contain many threading dislocation segments. For hetero-epitaxial films on fixed films, the weakest bonding surface positions are confined to narrow grid-line-like regions above the FF–HW boundary screw dislocations; Fig. 1. The nucleated half-loops would also be confined to these regions. Since each region is indefinitely long, a nucleated half-loop would be able to propagate indefinitely along the region length until they run out of the edge of the hetero-epitaxial film, thereby leaving no threading dislocation segments. For many half-loops nucleated in a given region, their threading dislocation segments will propagate

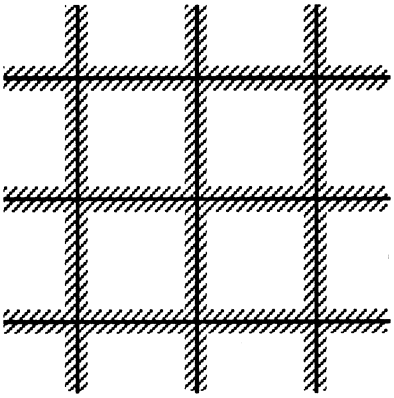

Fig. 1. Top view of the hetero-epitaxial film on the fixed film. Indicated are the underlying screw dislocation network at the boundary between the fixed film and the handle wafer owing to twist (*solid lines*), and the hetero-epitaxial film surface regions of high energy wherein the dilational misfit relief edge dislocations will be nucleated (*hatched regions*)

along the same line direction to meet each other, leading to their mutual annihilation. Thus, there will also be few threading dislocation segments left in the hetero-epitaxial film. This, together with the first possibility, is what the term *correlated* misfit dislocation generation refers to.

There is a quantitative requirement for fully relaxing the hetero-epitaxial film on a fixed-film substrate with few threading dislocations left. Namely, the underlying screw dislocation density must match or surpass that of the needed edge dislocation density. Assuming that the Burgers vectors of the edge and screw dislocations are of the same magnitude, we arrive at the condition

$$\Phi \geq \varepsilon\,, \tag{1}$$

where ε is the dilatational misfit given by $\varepsilon = (a_s - a_0)/a_0$, where a_s and a_0 are the stress-free lattice parameters of the fixed film and the epitaxial crystals, and Φ is the rotational misfit between the fixed-film and handle-wafer substrates defined as $\Phi = 2\sin\Theta/2$, with Θ being the twist angle. If (1) is not satisfied, i.e., $\Phi < \varepsilon$, there may be some threading dislocation segments in the heteroepitaxial film, since some of them must nucleate at random surface positions. For $\Phi = \varepsilon$ the density of the screw. and edge dislocations will be equal. For $\Phi > \varepsilon$, there will be a lack of edge dislocations on top of a fraction of the screw dislocations. It is interesting to note that (1) is satisfied in the work by Ejeckam et al.: in their $In_{0.35}Ga_{0.65}P$ hetero-epitaxial films the dilational misfit is $\varepsilon = 0.1$, and twist angles between the fixed films and the handle wafer GaAs substrates are 9°, 17°, and 32°, corresponding to $\Phi = 0.157$, 0.296, and 0.55, respectively.

The hetero-epitaxial film on a fixed film relaxed in such a way is not in its lowest energy state, because it contains the shear strain inherited from the fixed film produced by the screw dislocations at the FF–HW boundary . The fixed film is in a metastable state, and when kinetic conditions permit, the fixed film can realign itself to the exact handle wafer orientation by eliminating the screw dislocations, via dislocation climb or via generation of *un-twist* screw dislocations whose Burgers vectors are opposite to those of the initial misfit screw dislocations. The former can be achieved by high-temperature annealing, whereas the latter needs an applied stress at a fairly high temperature. The hetero-epitaxial film on top of the fixed film is a source of stress, leading to the possibility that after being fully relaxed, not only may the hetero-epitaxial film be free from (edge) threading dislocation segments, but the screw dislocation network underneath the fixed film may also have been eliminated. This requires the generation of screw dislocations also. The possible outcome of such a process is schematically illustrated in Fig. 2 For clarity, in Fig. 2 the heteroepitaxial film is shown to have a larger lattice constant than the fixed film. The small filled circles in Fig. 2 represent the top surface atoms of the fixed film, for which the shear displacement produced by the screw dislocations at the FF–HW boundary is indicated by dotted lines, which is shown to be asymmetric for two reasons: (i) for clarity; and (ii) the thin fixed film is expected to absorb most of the shear because of the screw dislocations. Also shown are two rows of large open circles representing the bottom surface atoms of the hetero-epitaxial film, indicating two different cases. In the top row only the effect of the misfit edge dislocation is shown. The shear displacement originating from the fixed film is still present in the hetero-epitaxial film. In the bottom row, effects of both the misfit edge dislocations and the un-twist dislocations are shown. In the hetero-epitaxial film, this represents: (i) the replacement of the elastic strain energy due to lattice mismatch by energy of the edge-type misfit dislocations at the interface of the two films; and (ii) the removal of the shear displacement originating from the fixed film. For clarity, what has not been shown in Fig. 2 is the fact that if the process of un-twisting is operational, it will also have removed the shear displacement in the fixed film.

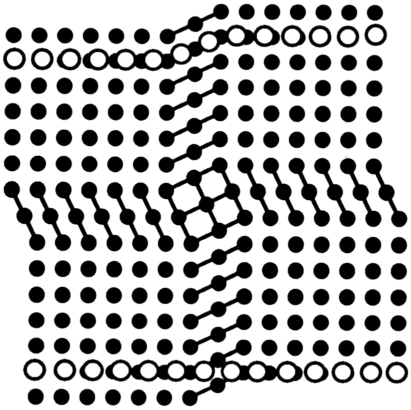

Fig. 2. Schematic diagram showing two possibilities for how the misfit elastic strain may be relaxed in the hetero-epitaxial film grown on a fixed film. See text for details

In summary, we have presented a tentative interpretation of the role of the fixed-film substrate for growing lattice mismatched hetero-epitaxial films with a low density of extended defects. The screw dislocation network at the fixed-film/handle-wafer boundary can getter away contaminants that would otherwise generate growth stacking faults. The same dislocation network could also provide confined regions for the nucleation of lattice-mismatch-relieving dislocations to occur without threading dislocation segments being left in the hetero-epitaxial film bulk region.

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