Effect of interface chemistry on the growth of ZnSe on the Si(100) surface

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Heteroepitaxial growth of compound semiconductors on Si surfaces is strongly affected by the chemical bonding at the interface. In this work, the growth of ZnSe on Si(100) surfaces by molecular-beam epitaxy has been investigated primarily by transmission electron microscopy (TEM). The dominant effect during interface formation is the tendency of Si and Se to react to form the amorphous compound $SiSe_2$. By utilizing a number of growth techniques, we have been able to characterize the interface reaction and will describe methods where the reaction can be minimized. For ZnSe films grown at elevated temperatures, TEM images show the presence of a thick (~ 100 nm) amorphous layer at the interface. For films deposited on Si(100) at room temperature and then crystallized by solid-phase epitaxy, we find no amorphous layer, but submonolayers of Se bonded to the Si surface may give rise to a misorientation between the Si and ZnSe crystals and to the large areas of twinned ZnSe that are observed. We discuss mechanisms for the tilt and for the observation that the twinned areas exist only in one of the two allowed configurations. The presence of an arsenic monolayer on the Si(100) surface prior to ZnSe growth is found to prevent any reaction between Si and Se and we find parallel epitaxial growth without any significant twinning. For growth of ZnSe either via room-temperature deposition and solid-phase epitaxy or on Si(100):As, we obtain very uniform films. This is in contrast to the situation for GaAs-on-Si epitaxy where island formation is dominant at comparable thicknesses. The use of ZnSe as an interlayer for GaAs-on-Si growth is proposed.

I. INTRODUCTION

Heteroepitaxy of compound semiconductors on elemental semiconductor substrates can lead to many promising applications such as the monolithic integration of optical and electronic functions in devices. The successful growth of a compound semiconductor on Si, however, requires many potential problems to be solved. Mismatch of the lattice constant and/or the coefficient of thermal expansion causes significant difficulties but, even in the case where there are no such mismatches, the chemical differences between the substrate and the overlayer can prevent good epitaxy. Such chemical differences can lead to several problems which need to be overcome. Undesirable three-dimensional growth tends to occur if there is relatively weak bonding between the overlayer species and the substrate atoms or if a surface-confined passivating layer is formed which has a low surface energy. In the opposite extreme, compound formation between atoms in the overlayer and those in the substrate leads to dissolution instead of controlled overlayer growth. In the well-studied case of GaAs on Si, the formation of a chemically inert monolayer of arsenic on the Si surface makes it difficult to form a two-dimensional GaAs layer. This occurs because the extra valence electron in the As atom compared to Si allows a monolayer of As to bond to the surface in such a way that all of the surface and interface bonds are saturated.[1,2] Bonding of GaAs to this inert template is thus difficult and is likely to be related to the tendency of GaAs to form islands in the initial stages of growth of GaAs on Si.[3] In the present work we have studied the growth of ZnSe on Si(100) using molecular-beam-epitaxy (MBE) techniques. Electron-counting arguments would suggest that a stable Se monolayer would terminate the Si(100) surface as is the situation for the analagous Ge(100):S case.[4–6] However, reactivity of Se and Si (to form volatile SiSe molecules[7]) and the ease of Se insertion into Si—Se bonds (which give rise[8] to a layer on the surface of disordered $SiSe_2$, the Se analog of SiO_2) make it difficult, if not impossible, to form a stable Si(100): Se monolayer.[8] Growth of ZnSe on Si(100) therefore presents the opposite problem from GaAs on Si, namely, the requirement that the Si-Se reaction be prevented or minimized.

Early results found that ZnSe could be grown successfully on Si with MBE by carefully controlling the Zn-to-Se flux ratio at the substrate.[9,10] Park and Mar[10] found that the best results could be obtained by slowly ramping up the Se flux while holding the Zn flux constant.[10] In the absence of any Se flux the sticking coefficient of Zn on the surface was found to be zero at the substrate temperature of 330 °C that was used. It was concluded that the growth must be initiated at a slow rate *and* that the flux of Zn should be greater than the Se flux at the initiation.[10] Epitaxial growth presumably occurred because the Zn layer prevented the Se and Si atoms from reaching one another and forming $SiSe_2$. An abrupt interface between Si(100) and the Zn layer of ZnSe(100), however, will have an interface dipole as discussed by Harrison *et al.*[11] A dipole such as this is energetically very unfavorable and is probably reduced in practice by atomic mixing at the interface.[11] As we describe below, we have found that the Zn prelayer is unnecessary if ZnSe is deposited at room temperature (RT) and then the layer is crystallized by solid-phase epitaxy (SPE). This is important for growth using a ZnSe evaporation source where a Zn-only flux is not possible. Following the suggestion of Chadi,[12] we have also found that a monolayer of As on

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the Si(100) surface allows the growth of ZnSe at substrate temperatures of around 300 °C, which are those typically used for MBE growth of ZnSe. Because the As monolayer reduces or eliminates the interface dipole, no intermixing between Si and Zn or Se is necessary at the interface. In the following sections we will present results for ZnSe grown on Si via a number of methods and discuss the effects of the chemical nature of the interface formed in each case. Transmission electron microscopy (TEM) will be utilized to examine the structure and orientation of the ZnSe layers.

II. EXPERIMENTAL DETAILS

The silicon substrates were cut from polished wafers (*n* type, 0.01 Ω-cm) and heated by passing a current through them. Unless otherwise noted, their surface normals were 4° from the [100] direction, with the tilt being towards one of the ⟨011⟩ directions. The samples were cleaned by standard solvent and acid dips and oxidized with a uv-ozone technique.[13] After introduction into the ultra high-vacuum (UHV) environment, they were outgassed for several hours by resistively heating to 600 °C and then the oxide layer was removed and the surface was ordered by annealing to 1030 °C for 2 min. The ZnSe growth and some of the characterization experiments were carried out in a multichamber system which allows samples to be transferred in UHV from a MBE chamber to other chambers containing Auger and x-ray photoelectron spectroscopies, scanning tunneling microscopy, and low-energy electron diffraction. The MBE chamber has a number of effusion cells, is pumped with ion and cryo pumps, and has liquid-nitrogen cold shrouds to maintain a clean ambient. The ZnSe was grown using an effusion cell containing the compound ZnSe and some of the earlier results for Se alone on Si that we refer to were obtained by utilizing an electrochemical Se cell.

After the layer growth and any subsequent annealing steps, the samples were removed from the UHV environment for TEM studies. The samples were then coated with a thin film of amorphous Si as a protective layer and thinned using standard methods for TEM cross sections.

III. RESULTS

A. ZnSe deposition on Si(100) at 300 °C

A TEM cross section typical of those for ZnSe films deposited at 250 °C–300 °C is shown in Fig. 1. We can observe that the surface layer is polycrystalline and is separated from the Si by an amorphous layer which contains small, randomly oriented crystallites. The composition of the polycrystalline surface layer was determined by Auger spectroscopy to be ZnSe. Previous soft-x-ray photoelectron spectroscopy (SXPS) measurements[8] on ZnSe films grown in this manner showed that Si and Se reacted during growth to form $SiSe_x$ compounds with a range of compositions including $SiSe_2$. This was revealed in the SXPS spectra by the presence of four equally spaced chemical shifts of the Si 2*p* core level.[8] Although we do not have direct evidence, the SXPS results and the

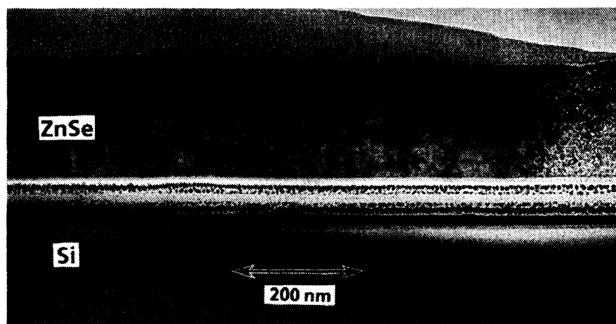

FIG. 1. TEM cross section in a ⟨011⟩ projection of a ZnSe film deposited on Si at 300 °C. An amorphous Si film has been evaporated onto the ZnSe layer to provide protection during TEM thinning. Electron diffraction showed the region marked as ZnSe to be polycrystalline.

TEM image suggest that the amorphous layer in Fig. 1 is $SiSe_x$ and that the included crystallites are Zn or ZnSe particles. Because the vapor pressures of Zn and Se are comparable, it is possible to have a wide variety of [Zn]:[Se] ratios in a film when Se-Si formation is taking place. Once ZnSe has nucleated, as it has above the amorphous layer, stoichiometry is maintained because, to a good approximation, the sticking coefficient of a Zn (Se) atom on the surface is 1 if it finds a Se (Zn) atom and 0 otherwise.[10]

B. ZnSe deposition at room temperature plus solid-phase epitaxy

The results described in the previous section suggest that kinetic barriers to the formation of the $SiSe_x$ (and/or the escape of SiSe molecules) need to be utilized if good ZnSe films are to be made. Lowering the substrate temperature reduces the ability of the system to get over any kinetic barrier and has been shown in many heteroepitaxial systems to enhance growth quality. We expect that once a ZnSe film is deposited approximately stoichiometrically, it may not be possible for large numbers of Se atoms to reach the Si because the Se atoms are tied down by bonding to Zn atoms. This would allow the RT-deposited films to be annealed and crystallized without any significant Si-Se interdiffusion and reaction taking place.

A series of ZnSe films was grown by room-temperature deposition followed by solid-phase regrowth. Low-energy electron diffraction was used to determine the degree of crystallinity of the films as a function of annealing temperature. It was found that annealing films for 2 min at 500 °C gave crystalline films without any significant reaction between the ZnSe and the Si substrate. Annealing at 600 °C did cause a reaction to take place. A cross-section TEM image of a 50-nm ZnSe film on Si(100) is presented in Fig. 2. There is no evidence for the formation of a thick amorphous layer between the Si and the ZnSe. The ZnSe film also has a characteristic orientation relative to the substrate. The inset in Fig. 2 shows the electron diffraction pattern that was obtained from the same area of the interface. Several conclusions can be

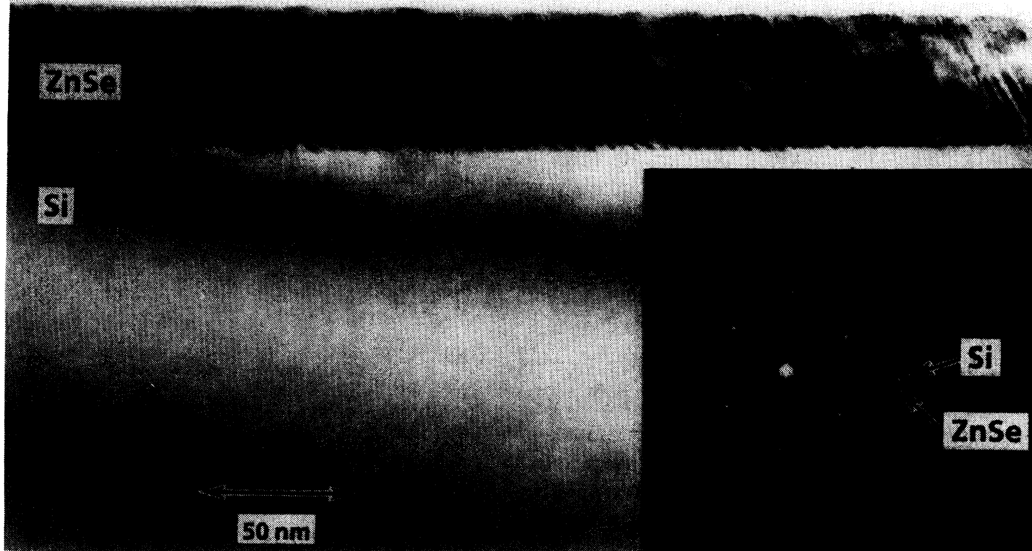

FIG. 2. TEM cross section, in a ⟨011⟩ projection, of a ZnSe film deposited on Si at room temperature and then annealed for 2 min at 500 °C. The [100] vector for the substrate is 4° from the interface normal and has a component towards the right of the figure. The inset is an electron diffraction pattern of the same area.

drawn from the figure: (i) the film is uniform in thickness (this is also found to be the case for thinner ZnSe films prepared with the same method); (ii) the diffraction pattern shows that the ZnSe crystal is tilted with respect to the Si substrate; and (iii) a large number of crystal defects tilting from the lower right to the upper left of the film are seen. An atomic resolution image of a similarly prepared sample is shown in Fig. 3. Here, the angle between the Si and ZnSe axes can be measured directly and is found to be close to 6°. The fact that we can simultaneously see the atomic structure of both the Si and ZnSe implies that the two crystals are oriented parallel to one

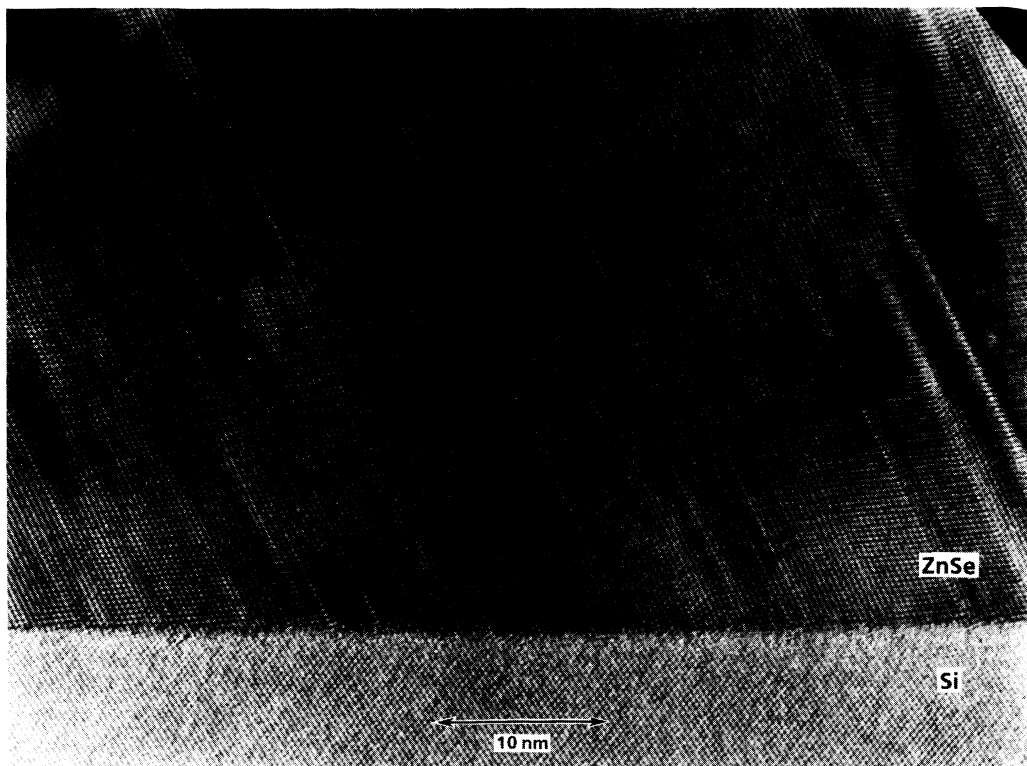

FIG. 3. High-resolution TEM cross section, in a ⟨011⟩ projection, of a ZnSe film deposited on Si at room temperature and then annealed for 2 min at 500 °C. The [100] vector for the substrate is 4° from the interface normal and has a component towards the right of the figure.

another in the plane perpendicular to the image (i.e., in the [011] direction). The orientation between the two crystals and the surface offcut is shown schematically in Fig. 4(a). The misorientation angle was measured for a number of films deposited in the same manner and was found to be 5°±1° with the same orientation sense relative to the surface offcut in all cases. A film grown on a 1.5°-offcut substrate also had a 4° misorientation showing that the misorientation was insensitive to the offcut angle.

Also revealed in the high-resolution image are a number of stacking faults or microtwins. The second characteristic of all of the ZnSe films prepared by RT deposition and solid-phase epitaxy is the fact that all of these stacking faults are oriented on one of the two possible sets of {111} planes imaged in a ⟨011⟩ direction. Figure 4(a) shows the orientation of the stacking faults relative to the interface. It can be seen in the high-resolution image of Fig. 3 that there are comparable areas of ZnSe that are twinned and untwinned relative to the Si crystal axes. A predominance of one of the sets of twin planes over the other has been found at large distances from the interface for GaAs on Si.[14,15] There are several differences between the observations we have made and those in the GaAs-on-Si case. There was no misorientation observed for GaAs on Si and the ratio of the majority to minority stacking faults was 10:1 for GaAs on Si and is at least 200:1 in our case where we have not observed any minority orientations in any of our films.

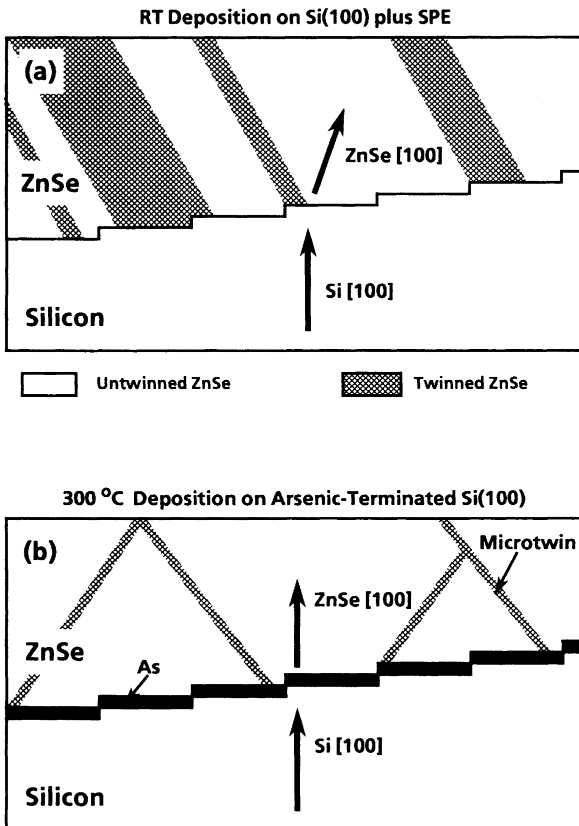

FIG. 4. Schematic cross section, in a ⟨011⟩ projection, showing the relative orientations of the ZnSe and Si crystals, the stacking faults, and the surface steps at the interface for (a) a film deposited on Si(100) at room temperature and then annealed at 500 °C for 2 min and (b) for a film deposited on arsenic-terminated Si(100) at 300 °C. The areas of twinned ZnSe are shown by crosshatching.

C. ZnSe growth on Si(100):As

On the basis of electron-counting arguments, Chadi[12] suggested the use of a single As monolayer between Si and ZnSe. Such a monolayer allows all bonds to be fully occupied on both sides of the interface. With the assumption that the bulk Si and ZnSe materials are fully coordinated, then Zn, Si, and Se atoms contribute $\frac{1}{2}$, 1, and $\frac{3}{2}$ electrons, respectively, per bond both in the bulk and at the interface. A ZnSe crystal has alternating layers of Zn and Se atoms in the [100] direction with two bonds per atom between layers. Without an As interlayer and with a Si-Se interface (i.e., an atomic plane sequence of -Si-Si-Si-Se-Zn-Se- in the [100] direction) then each Se atom at the interface is surrounded by two electrons from the Si layer, one electron from the Zn layer above, and six electrons itself for a total of nine, or one electron in excess of the energetically favorable octet configuration. Conversely, in the -Si-Si-Si-Zn-Se-Zn- case, the interface Zn atom has a total of seven electrons for four bonds, or one too few. With an As monolayer and a sequence of -Si-Si-Si-As-Zn-Se-Zn-, the As layer has two electrons from the Si layer below, one electron from the Zn layer above, and five electrons itself for a total of eight electrons. The As monolayer therefore allows all bulk and interface atoms to be fully coordinated.

The As monolayer was made by exposing the clean, ordered Si(100) surface to an As_4 flux while increasing its temperature from RT to 650 °C, holding at that temperature for 20 s and then dropping the sample temperature back to RT. This has been shown previously to give rise to a monolayer of As with the As-As dimers of the surface layer being aligned perpendicular to the step edges of the Si substrate.[16] The results of growing ZnSe on this Si(100): As surface at $T_s = 300$ °C are shown in Fig. 5. We see no evidence of any amorphous layer and find that the ZnSe is epitaxial on the Si substrate and is of uniform thickness. There are several notable differences compared to the RT deposition plus SPE films such as that shown in Fig. 2: (i) there is no discernible misorientation between the Si and ZnSe crystals, (ii) no large areas of twinned ZnSe are present, rather microtwins are present, and (iii) the microtwins occur on both possible {111} planes. We checked that these differences were due to the presence of As and not the SPE mechanism by carrying out a RT deposition on Si(100):As followed by a 500 °C anneal. The results were the same as those for growth on Si(100):As at 300 °C. The comparison between the two deposition methods is shown schematically in Figs. 4(a) and 4(b). Overall, the quality of the ZnSe grown on As-terminated Si(100) appears to be the most promising.

FIG. 5. High-resolution TEM cross section, in a ⟨011⟩ projection, of a ZnSe film deposited on arsenic-terminated Si(100) at 300 °C. The [100] vector for the substrate is 4° from the interface normal and has a component towards the left of the figure.

IV. DISCUSSION

The results described in the previous section show that the manner in which the ZnSe-on-Si(100) interface is formed can dramatically alter the subsequent growth of the ZnSe. The dominant effect appears to be the tendency for Si and Se to react to form a $SiSe_x$ compound. When Se is free to react with Si as is the case in Sec. III A, a thick amorphous $SiSe_x$ layer can form which disrupts the epitaxial template and leads to polycrystalline growth of ZnSe. At the other extreme of growth on As-terminated Si(100), the ability of all of the interface atoms to be fully coordinated prevents the compound formation. Another way of looking at this effect is to note that Se has a lower sticking coefficient to Si(100):As than does Zn and so a Zn layer can form, isolating the Se from the Si substrate. [By contrast, the results described in Sec. III A strongly suggest that Se has a greater sticking coefficient than Zn on clean Si(100), leading to $SiSe_x$ compound formation.]

We now turn to the intermediate case of RT deposition plus solid-phase epitaxy. The two effects that are unexpected are the tilt of the ZnSe lattice with respect to the Si lattice and the presence of areas of only one of the two possible twin orientations. As summarized in Fig. 4, the twin boundaries are oriented "downhill" relative to the offcut direction of the crystal. Tilts have been seen in many heteroepitaxial systems grown on offcut substrates, but none of the simple models for their origin seems to explain the present data. Lattice mismatch is not the only important parameter because (i) no tilt occurs for ZnSe growth on Si(100):As and (ii) results for GaAs on Si substrates are very different from those which we have described for ZnSe on Si, despite the fact that these two systems have close to the same mismatch. The tilts for GaAs on Si are in the opposite direction to those found here (i.e., the [100] vector of the ZnSe is tilted towards the surface normal for GaAs on Si and away from the normal for ZnSe on Si) and the tilts have a magnitude in the range of $0°-0.3°$ for GaAs on Si (see Refs. 17–20, for example), which is much smaller than the values of $5°\pm1°$ that we have measured in our ZnSe-on-Si films. We also note that ZnSe grown on Ge tilted by 4° (lattice mismatch $\sim0.2\%$) has a tilt of 0.5° in the same direction[21] as our results for ZnSe on Si. Because of the large magnitude of the tilts that we observe, we can rule out naive models in which the tilt is caused by a strain of the overlayer at the interface, but neither the substrate nor overlayer have dislocations. In order to obtain a 5° misorientation within such a model, the strain in the growth direction would be comparable to the substrate step height every step. Such a large distortion is unphysical. The tilt is much more likely to involve dislocations at the interface and these can be seen in Figs. 2 and 3. The observations that all of the observed stacking faults tilt in one direction relative to the offcut and that the overlayer is misoriented for the RT plus SPE growth and the fact that neither of these effects occurs for growth on Si(100):As suggest that the presence of the stacking faults and the crystal misorientation may be related.

Examination of the high-resolution image of Fig. 3 shows that the (111) planes of the twinned areas make a small angle with the substrate surface plane. The angles involved are shown in Fig. 6 where γ is the offcut angle of the substrate and β is the misorientation between the ZnSe and Si crystals. We have been unable to determine whether the ZnSe crystal is oriented with its [011] or [0$\bar{1}$1] direction parallel to the step edges of the interface for films deposited by RT deposition plus SPE. This leads to an ambiguity about the definitions of the various planes and we have therefore labeled the planes in Fig. 6 as $(111)_X$ and $(111)_Y$ for ease of discussion. The twins that are observed occur via a 180° rotation about the normal to the ZnSe$(111)_X$ plane and no twins are found to arise from rotations about the normal to the ZnSe$(111)_Y$ plane. The twins that are observed are denoted as ZnSe$(111)_Y$ (twin) and the twins which are not observed are ZnSe$(111)_X$ (twin). The angle between a twin {111} plane and the (100) surface where there is no crystal offcut and no misorientation is $70.5°-54.7°=15.8°$. [The angle between a (100) surface and the $(11\bar{1})$ plane is 54.7° and the angle between the $(1\bar{1}1)$ and $(11\bar{1})$ planes is 70.5°.] If we now take into account the crystal offcut and the misorientation, the angle α between the observed twin plane and substrate surface is given by

$$\alpha=15.8°-\beta-\gamma ,$$

where β and γ are defined to be positive. For the offcut angle of 4° and the tilt angle of 5° that are observed, we get $\alpha=7°$. Note that the equivalent angle for the unobserved twin plane would be given by $15.8°+\beta+\gamma$, or 25°. This result suggests that it may be advantageous for (111) planes of ZnSe to be nearly parallel to the substrate surface plane. There are several plausible reasons for this to be the case and these will be discussed below.

The first point to remember is that there is no misorientation or large fraction of twinned ZnSe for growth on the Si(100):As surface, independent of whether the deposition is at 300 °C or at RT followed by SPE. This strongly suggests that the mechanism responsible for these effects during the RT deposition plus SPE on clean Si(100) is related to the reaction of Se with the substrate. We know from SXPS results[8] that Se can react with the Si substrate either to give a thick $SiSe_x$ layer or to terminate the Si(100) surface with at least a partial monolayer of Se atoms in fully coordinated bridge sites (Fig. 7). The TEM images in Figs. 2 and 3 rule out the presence of thick amorphous layers at the interface, but it is possible that part of the substrate has a nonreactive Se monolayer such as that shown in Fig. 7. If a fully coordinated Se monolayer is formed on the Si surface during the initial stage of SPE, then bonding of the ZnSe to it would be weak. In that case the ZnSe will not have a seed to recrystallize from and it is possible that ZnSe crystallites will form with their lowest energy face parallel to the interface. The TEM image would then suggest that the ZnSe prefers to be oriented with one of its {111} faces parallel to the interface. At the same time, some areas of the Si substrate will not be covered by a Se layer and will provide a seed for the (100) growth of ZnSe. In order to accommodate both of these orientations, the ZnSe tilts with respect to the Si crystal to share the strain equally between the twinned and untwinned regions. With the observed tilt angle of 5° this means that the (100) ZnSe regions are tilted by 5° from the Si(100) planes and the {111} faces of the twinned regions make a 7° angle with the interface. Assuming that the as-deposited film has comparable probabilities for Si-Se and Si-Zn nearest neighbors, then the areas of the interface that give rise to twinned and untwinned ZnSe might also be comparable.

Other explanations do not involve the reactivity of Si and Se. For the case of laser-assisted growth of GaAs on Si, Lao *et al.*[15] found that the majority of stacking faults far away from the interface had the same orientation relative to the offcut direction of the substrate as we have described here. They were unable to characterize the ratio of the two stacking faults at the interface, but assumed that those too had a preferential orientation. They examined atomic models of the interface formed for both the majority and minority twin structures and found slight differences which could, in principle, lead to a favoring of one orientation over the other. Because there was no misorientation between the GaAs and Si crystals, the mechanisms are probably different for ZnSe on Si.

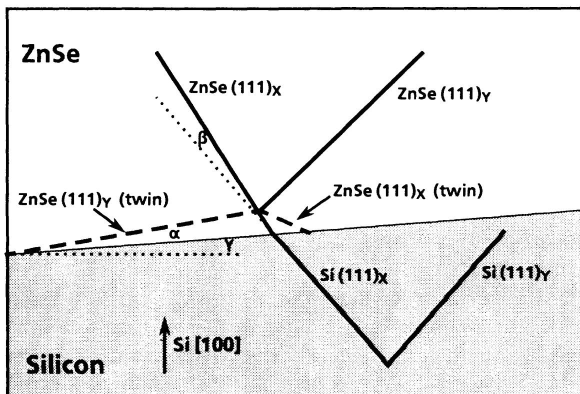

FIG. 6. Schematic cross section, in a ⟨011⟩ projection, for a film deposited on Si(100) at room temperature and then annealed at 500 °C for 2 min. The {111} planes normal to the cross-section plane are shown end on for Si and for ZnSe. The two possible twin {111} planes are shown for ZnSe. The twin plane marked "ZnSe$(111)_X$ (twin)" has not been observed in any of the films prepared by RT deposition and SPE.

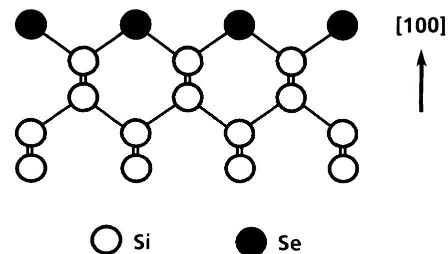

FIG. 7. Schematic atomic structure of Si(100):Se. In this structure, all of the Se and Si atoms in the surface region are fully coordinated.

V. CONCLUSIONS

The growth of ZnSe on Si is complicated by the tendency of Si and Se to react to form an amorphous layer of $SiSe_x$. This effect has been investigated in detail by characterizing the effects of different growth methods on the interface structure and on the properties of the ZnSe film within ~20 nm of the interface. As a result, we have found two alternative methods to avoid or minimize the effect of the interreaction. The first of these prevents the intermixing by depositing ZnSe at room temperature and then solid-phase recrystallizing it. The second uses a monolayer of As to prevent the reaction of films grown at elevated temperatures. In the case of the RT deposition plus SPE, the reaction between Si and Se may only affect the first monolayer, but be manifested by the presence of large areas of twinned ZnSe.

The advantages of growth on Si(100):As then appear to be twofold: there is no tilt between the substrate and the ZnSe film, and the films have similar numbers of stacking faults in the two possible orientations allowing microtwin annihilation to take place. The RT deposition on clean Si(100) plus SPE also gives rise to a large fraction of twinned ZnSe.

The ZnSe films produced by (i) room-temperature deposition and SPE and (ii) deposition on arsenic-terminated Si(100) are particularly uniform. By contrast, GaAs films grown directly on Si are very nonuniform at comparable thicknesses and the growth is dominated by island formation and coalescence.[3] Because of the uniformity of the ZnSe-on-Si films and the close lattice match between GaAs and ZnSe, films of ZnSe are promising as interlayers for GaAs-on-Si growth.[22–24] Our results[24] for thin MBE-grown layers showed that uniform GaAs films could indeed be grown on ZnSe on Si at thicknesses at which island formation would take place if no ZnSe interlayer was present. In addition, ZnSe has a lower plastic deformation threshold than GaAs (the Knoop hardness for Si, GaAs, and ZnSe is 1150, 750, and 150, respectively). The value of a ZnSe interlayer would be that the dislocations arising from the lattice mismatch between ZnSe and Si would be confined, either during the growth or during subsequent annealing, to the softer ZnSe and not propagate into the GaAs overlayer.[22] We note that thick GaAs layers grown with metalorganic chemical vapor deposition on ZnSe-on-Si films have been found to be of better quality than those grown on bare Si.[23]

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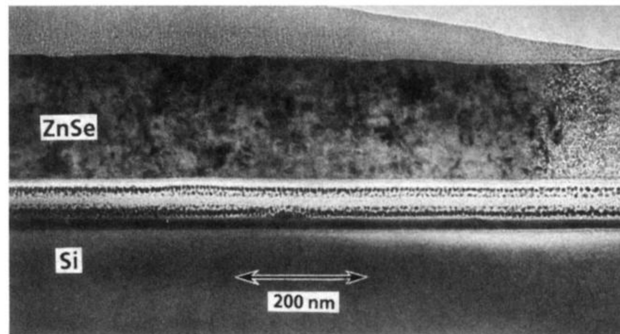

FIG. 1. TEM cross section in a ⟨011⟩ projection of a ZnSe film deposited on Si at 300 °C. An amorphous Si film has been evaporated onto the ZnSe layer to provide protection during TEM thinning. Electron diffraction showed the region marked as ZnSe to be polycrystalline.

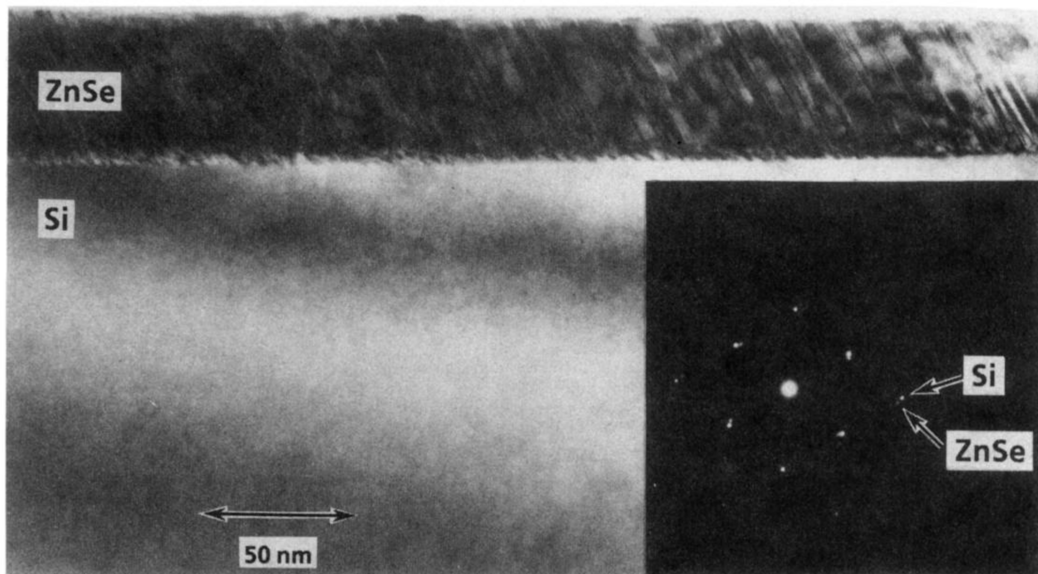

FIG. 2. TEM cross section, in a ⟨011⟩ projection, of a ZnSe film deposited on Si at room temperature and then annealed for 2 min at 500 °C. The [100] vector for the substrate is 4° from the interface normal and has a component towards the right of the figure. The inset is an electron diffraction pattern of the same area.

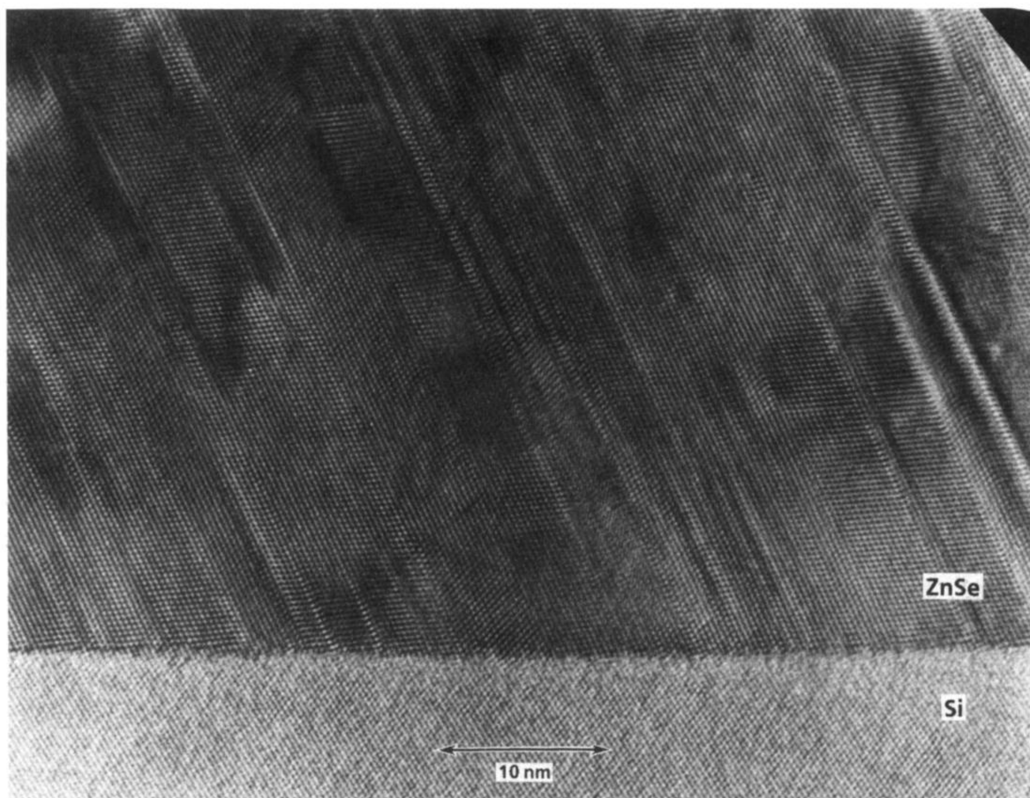

FIG. 3. High-resolution TEM cross section, in a ⟨011⟩ projection, of a ZnSe film deposited on Si at room temperature and then annealed for 2 min at 500 °C. The [100] vector for the substrate is 4° from the interface normal and has a component towards the right of the figure.

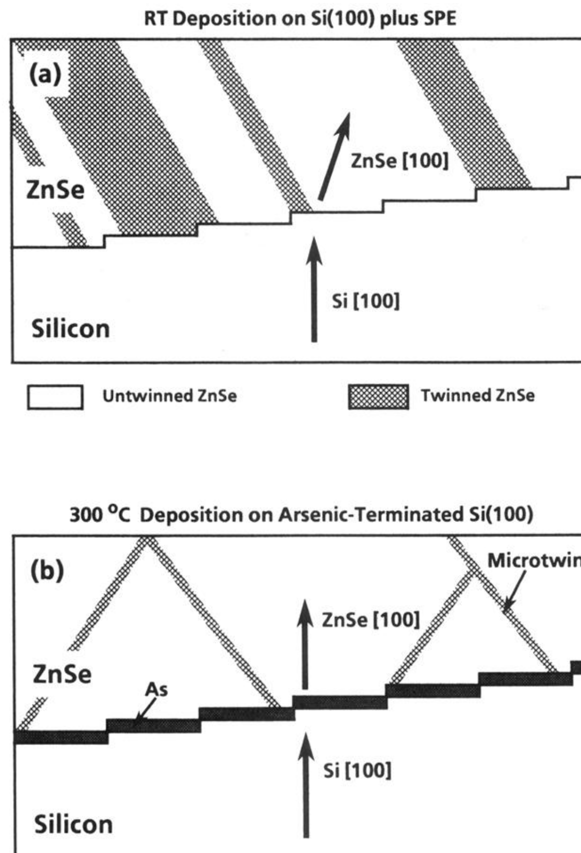

FIG. 4. Schematic cross section, in a ⟨011⟩ projection, showing the relative orientations of the ZnSe and Si crystals, the stacking faults, and the surface steps at the interface for (a) a film deposited on Si(100) at room temperature and then annealed at 500 °C for 2 min and (b) for a film deposited on arsenic-terminated Si(100) at 300 °C. The areas of twinned ZnSe are shown by crosshatching.

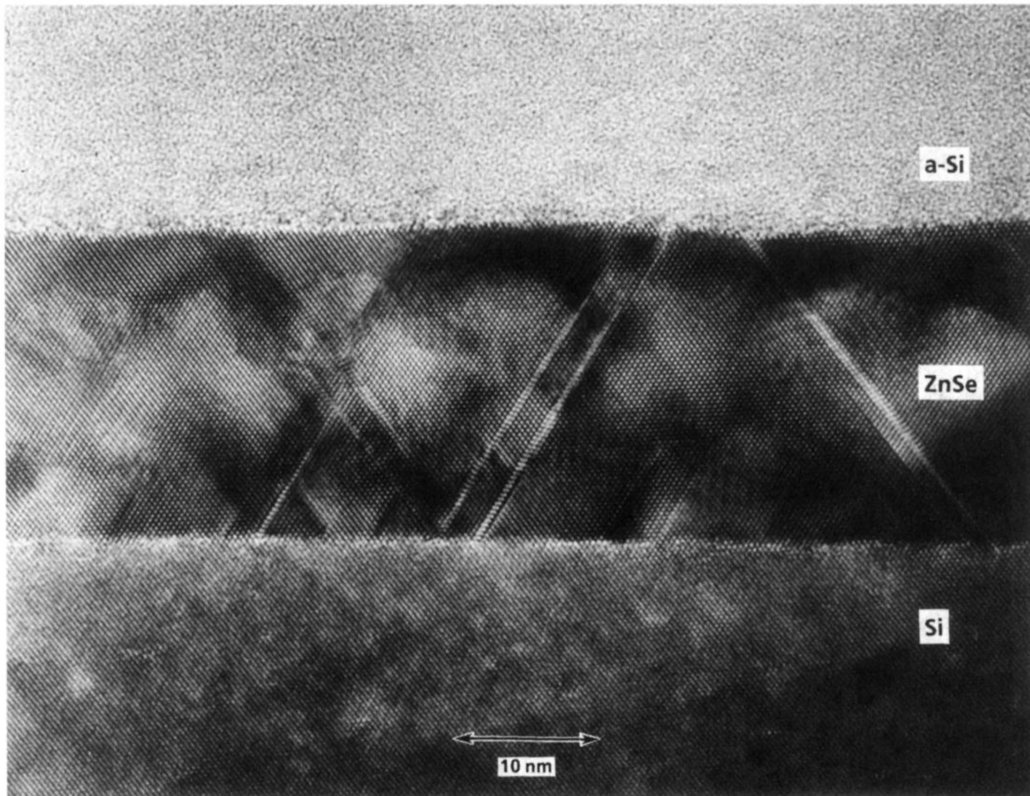

FIG. 5. High-resolution TEM cross section, in a ⟨011⟩ projection, of a ZnSe film deposited on arsenic-terminated Si(100) at 300 °C. The [100] vector for the substrate is 4° from the interface normal and has a component towards the left of the figure.

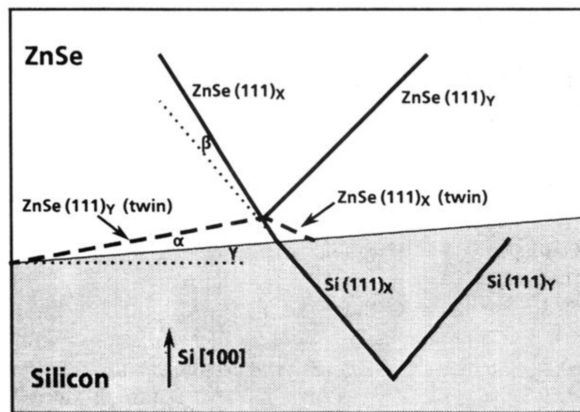

FIG. 6. Schematic cross section, in a ⟨011⟩ projection, for a film deposited on Si(100) at room temperature and then annealed at 500 °C for 2 min. The {111} planes normal to the cross-section plane are shown end on for Si and for ZnSe. The two possible twin {111} planes are shown for ZnSe. The twin plane marked "ZnSe$(111)_X$ (twin)" has not been observed in any of the films prepared by RT deposition and SPE.

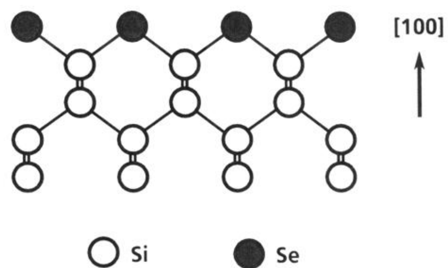

FIG. 7. Schematic atomic structure of Si(100):Se. In this structure, all of the Se and Si atoms in the surface region are fully coordinated.