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Surface dimerization induced CuPt_B versus CuPt_A ordering of GaInP alloys

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Using a valence force field approach and *ab initio* pseudopotential calculations, we examine the role of subsurface strain in the ordering of $Ga_{0.5}In_{0.5}P$ alloys. We show that depending on the orientation of the surface phosphorus dimers, these alloys can have ~i! a CuPt_A ordering for 1×2 or *c*~4×4! reconstruction; ~ii! a CuPt_B ordering for 2×1 or *b*2~2×4! reconstruction; and ~iii! a triple period ordering for 2×3 or *c*~8×6! reconstruction. These results are in good agreement with recent experiments of Gomyo *et al.* @Phys. Rev. Lett. **72**, 673 ~1994!; Jpn. J. Appl. Phys. **34**, L469 ~1995!#. © *1995 American Institute of Physics.*

Spontaneous ordering of III–V alloys has now been extensively observed and characterized in many semiconductors.[1] The most frequently seen spontaneous ordering consists of monolayer superlattice alternation along the ^111& cubic body diagonals.[1] Of the four bulk-equivalent body diagonals, ordering has been seen to take place along only two directions ~@111# and @111#, called CuPt_B variants!, while, until recently, ordering along the other two directions ~@111# and @1 11#, called CuPt_A variants! was absent. Theoretical studies[2–4] have demonstrated the relationship between surface reconstruction and spontaneous ordering in the 2D surface plane. It was shown that a cation-terminated 2×2 surface reconstruction leads to a 2D CuPt_B ordering in the top surface layer and in the fourth subsurface layer, while an anion-terminated 2×1 reconstruction leads to strong CuPt_B ordering in the third subsurface layer. The occurrence of ordering in these layers, depending on reconstruction type, illustrates the intimate relation between top surface growth morphology and the depth of the ordering layer. It was further shown[4] that the main thermodynamic driving force for ordering is the creation of a subsurface selectivity for occupation by a small atom ~Ga! *under* the strained dimer rows, and occupation by a large atom ~In! underneath the opening *between* dimer rows. This subsurface selectivity induced by the top surface dimers depends naturally on the *dimer orientation.* The latter changes with reconstruction pattern. The subsurface selectivity in a given layer further depends on the depth of this layer under the top surface. Thus, nonflat surfaces can have a corresponding range of depths of subsurface ordering.

Several significant experimental observations were recently made in this respect. First, Gomyo *et al.*[5] discovered, under MBE growth conditions favoring an anion-rich 2×3 surface reconstruction, a *triple* period ordering of $Al_{0.48}In_{0.52}As/InP(001)$, in *either* the @111# *or* the @1 11# diblende GaP, InP, GaAs, and InAs. In the case of P double layers, we assume that the interlayer force constants involving surface P atoms ~which assume the positions of cations in the normal zinc-blende stacking! and first subsurface layer P atoms ~which assume the positions of anions in the zinc-blende stacking! are given by the average force constants of bulk zinc-blende GaP and InP. We have tested this assumption for the c~4×4! surface by comparing to first-principles pseudopotential results. The agreement is within a few hundredth of an angstrom for atomic positions and a few meV/surface atom for energies for displacement amplitudes of <0.5 Å.

Figure 1~c! shows the relative energies of various ordered 2D structures of $\mathrm{Ga}_{0.5}\mathrm{In}_{0.5}\mathrm{P}$ ~illustrated in Fig. 2! placed at the $Y=$third, second, and second subsurface layer, respectively, for the 2×1, 1×2, and 2×3 surfaces. Negative energies in Fig. 1~c! mean stable structures. A 2×2 superperiodicity is used in Fig. 2~a! for the 2×1 and 1×2 surfaces, but not for the 2×3 surface. A primitive 2×3 surface cell has ten different occupation patterns. Some of them are degenerate. Here, we show in Fig. 2~b! the five nondegenerate patterns: T1, T2, CuPt_B, NT1, and NT2. Out of the five, only T1 and T2 may evolve into triple period ordering in the @110# direction. We observe from Fig. 1 the following. ~i! The 2×1 surface exhibits a strong CuPt_B ordering at the third subsurface layer ~ordering energy $\mathrm{D}E_{\mathrm{ord}}=88$ meV/surface atom!. The ordering direction is @1 neighbor atoms in their normal tetrahedral positions, but at the surface they form dimers and are thus displaced towards each other by a sizeable amount ~ ; 0.8 Å each!. This creates a compressive strain on the subsurface layer atoms lying directly below the dimer rows