Electronic Structure of "Sequence Mutations" in Ordered $GaInP_2$ Alloys

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(Received 27 May 1999)

The electronic consequences of layer thickness fluctuations in CuPt-ordered $GaInP_2$ (layer sequence Ga-In-Ga-In...) are investigated. We show that the formation of a "sequence mutated" Ga-In-In-Ga... region creates a hole state $h1$ localized in the In-In double layer, while the electron state $e1$

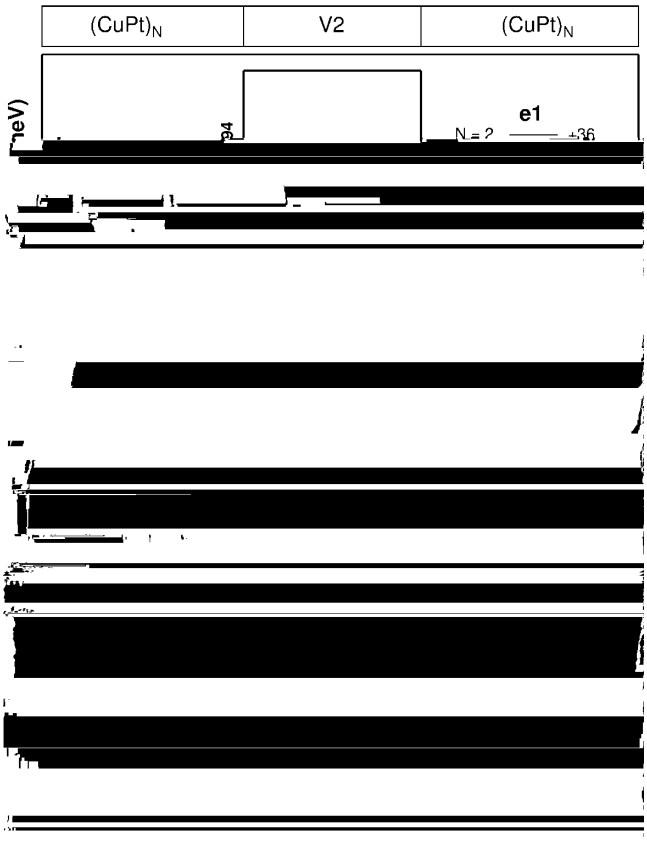

FIG. 3. The EPM calculated band edge energies for $(\mathrm{CuPt})_N$-$V2$-$(\mathrm{CuPt})_N$ structures (N is the thickness of CuPt region surrounding $V2$ region). The energies are in meV. The LDA-calculated band offset between CuPt and $V2$ for conduction band minimum (valence band maximum) is 150 (56) meV, confirming the type-II alignment predicted by EPM. For $N = 2$ the LDA-calculated value for $\Delta = h1 - h2$ is 80 meV, verifying the EPM predicted appearance of $h1$ level above $h2$. The lower panel shows the $e1$, $h1$, and $h2$ wave functions squared for the $N = 5$ system.

insensitivity to the presence of Ga-Ga segment is expected, since the Ga-Ga double layer acts as a barrier (Fig. 3), and thus does not play an important role for the band edge localization. The lowest conduction state $e1$ remains localized in the CuPt region as shown in the lower panel of Fig. 3, and its energetic position approaches the conduction band minimum of CuPt as the thickness N of the CuPt region surrounding $V2$ is increased. The important observation emerging from Fig. 3 is that the occurrence of a sequence mutation in the form of an In-In layer in the CuPt structure creates a spatially *indirect, low-energy* transition (from $e1$ to $h1$), in addition to the spatially direct, excitonic transition (from $e1$ to $h2$).

To see the strength of various transitions, Fig. 3 shows the calculated dipole matrix elements $p = \langle \psi_{e1} | \hat{p} | \psi_{h1,h2} \rangle^2$ between these states, normalized with respect to the $e1$-$h1$ (band gap) transition in pure CuPt. Since the $e1$-$h1$ transition is spatially indirect, we find that its transition probability is smaller than for the spatially direct transition $e1$-$h2$. However, the $e1$-$h1$

smaller $\eta \sim 0.5$ [7]. To mimic this situation, the In layers are replaced by random $In_{0.5+\eta/2}Ga_{0.5-\eta/2}$ layers and the Ga layers are replaced by random $In_{0.5-\eta/2}Ga_{0.5+\eta/2}$ layers. Our calculations show that when $\eta = 1$ is changed to $\eta = 0.5$ the $h2$ (CuPt-confined) state energy drops by 53 meV, while h