



Electronic structure induced by lateral composition modulation in GaInAs alloys

H. A. Uhlir, U. Z. @, 6Y. UJWYz@!K "K Ub[žUbX'5'YI 'Ni b[Yf'

7 JhUjcb. 5dd'jYX'D\ng]Mj'@YHfYg'72ž&% ('f% - , l/Xc]. '%\$"%\$*' #6"%&% '\$'

J JYk 'cb]bY. \hnd.#Xl "Xc]cf[#f\$"%\$*' #6"%&% '\$'

J JYk 'HUV'Y'cZ7 cbHYbq. \hnd.#gVhUjcb"U]d"cf[#lcbYbhU]d#ci fbU#Ud'#&#%+3j Yf1dXZVtj

Di V]g\YX'VmiH'Y'5-Di V]g\]b[

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8Ybg]miž bVhcbU' hYcfmgja i Ujcbg'cZUa cfd\ci g\][\! 'cl]Xyg'cb'U'Vta dci bX'gYa]VtXi Vtcf'U'cm'U! 5'&C' #b; U5gf%\$\$Hf(³ &lžU! < Z &#b; U5gf%\$\$Hf(³ &lžUbX'U'NfC &#b; U5gf%\$\$Hf(³ &lž >"7\Ya "'D\ng"135ž&((+\$) f&\$%&l/%\$"%\$*' #6" *) +(' - '

9ZVhCZ]bHYfZJW' gfhi Vh fY'cb'hY'cdh]W' dfcdYfh]Yg'cZ'b5g# UGV'Ugyf'UWj Y'fY[]cbg' 5dd"'D\ng"'@YHf'80ž%*, ' f&\$%&l/%\$"%\$*' #6%() * & , '

H\YcfYh]W' dYfZ'fa UbW' UbX'gfhi Vh fY'cdh]a]hUjcb'cZ' ") (") ' a ' b; UGV#b; U5'GV'a i 'h'd'Y!ei Ubh a !k Y'' Ugyfg' 5dd"'D\ng"'@YHf'78ž&* (\$ f&\$%&l/%\$"%\$*' #6% * - % (* '

H\Y'gfhi Vh fUžVX'Ya]W'žUbX'Y'YVhcb]WdfcdYfh]Yg'cZU'ghUV'Y'; UG# U5g]bHYfZJW' >"5dd"'D\ng"'86ž* - (\$ f% - - l/%\$"%\$*' #6" +%+* '

6UbX'gfhi Vh fY'UbX'Vtzb]bYX'YbYf[m'Y] Y'g'cZ'hY'G]' ' B (#G]# U5g'gng]Ya ' >"5dd"'D\ng"'82ž&+) f% - +l/%\$"%\$*' #6" *) , \$, '

$\bar{1}10$ oriented atomic rows for each $\bar{0}01$ plane. In this in-plane view we see contraction of the inter-row distance in the Ga-rich region $\bar{1}$ and an equivalent expansion in the In-rich region 1 . This is consistent with the smaller covalent radius of Ga relative to the In atom. Surprisingly, all $\bar{0}01$ planes behave nearly identically, i.e., the $\bar{1}10$ in-plane displacements are *vertically phase-locked* between the different $\bar{0}01$ planes despite the changing composition of

gap reduction of ; 16 meV, indicating that the pure SPS structure induces a significant contribution to the redshift. Our calculations further reveal that the dependence of the redshift on CM wavelength l is rather weak. On the other hand, the redshift *increases* as one goes from sinusoidal lateral modulation to square-wave lateral modulation (; 10 meV for A ; 16%), and as one goes from integer-period SPS to fractional-period SPS -for $n=2$ SPS with the same CM parameters as for SPS $n=1.5$ we find a ; 5 meV smaller redshift!.

Effect of CM on polarization: -i! For pure $n=1.5$ @01# SPS we find the transition from the CBM to $V_1(V_2)$ to be polarized in the @110# ~@110# direction. The transition probability to V_3 is small, and thus @01# polarization should not be detected among these lowest energy transitions. On the other hand, -ii! a pure @110#

V_2-V_3 valence band splitting are 16 and 14 meV for $A = 16.7\%$ and increase with A . For $A=0$ ~representing a $n = 1.5$ SPS with no CM where the mixed GaIn layer is randomly occupied! the corresponding splittings are 4.1 and 1.3 meV. Figure 3 shows that CM+SPS act to raise the valence bands, lower the conduction band, and hence reduce the band gap. The calculated band-gap redshift for $l = 149 \text{ \AA}$, $u = @110\#$ and $n=1.5$ is shown in Fig. 3-a!; it is ; 40 (80) meV for A ; 8 (16)%. For $A=0$ ~SPS only! we find a band-