



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

J Jk 'HUV'Y'cZ7 cbHYbq. \hnd.#gVhUjcb"U]d"cf[ #f\$"%\$\*' #6%&% '\$'

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

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8Ybg]miž bVfcbU' hYcfmg]a i Ujcbg'cZUa cfd\ci g\][ \! 'cl ]Xyg'cb'U'Vta dci bX'gYa ]VtbXi Vtcf'U'cm'U! 5'&C' #b; U5gf%\$ \$f( 3 &žU! < Z &#b; U5gf%\$ \$f( 3 &žU'U'NfC &#b; U5gf%\$ \$f( 3 &ž >"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 'hd'Y!ei Ubh a !k Y' 'Ugyf' 5dd'"D\ng"'@YHf'78ž&\* ( \$ f&\$%&l/%\$"%\$\*' #6% \* - % ( \* ' '

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

6UbX'gfhi Vh fY'UbX'VtbZ]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  $\sim 16$  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  $\lambda$  is rather weak. On the other hand, the redshift *increases* as one goes from sinusoidal lateral modulation to square-wave lateral modulation ( $\sim 10$  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  $\sim 5$  meV smaller redshift!).

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

$V_2-V_3$  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  $\lambda = 149 \text{ \AA}$ ,  $\mathbf{u} = \Gamma$  and  $n=1.5$  is shown in Fig. 3-a; it is  $\sim 40$  (80) meV for  $A = 8$  (16)%. For  $A=0$  (SPS only) we find a band-