Band structure and stability of zinc-blende-based semiconductor polytypes

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Using a first-principles generalized one-dimensional Ising model we have studied the band structure and stability of two types of zinc-blende-based polytype series: type-a $GaInP_2$ and type-b $CuInSe_2$. The interaction parameters for the formation energy are found to be short range, while the convergence is slower for the band-gap and conduction-band energies of the type-a $GaInP_2$ polytypes. We predict that the CuAu-like phase can coexist in nominally chalcopyrite $CuInSe_2$ and $CuInS_2$, while such coexistence is less likely in $CuGaSe_2$. We also predict that type-II band alignment can exist between different ordered type-a $GaInP_2$

A_3B and AB_3 tetrahedral clusters around the common C atom [Figs. 1(a) and 1(b)]. In the type-b plane

method,[20] the total-energy, band-gap energy and the energy lineups of the valence-band maximum (VBM) and conduction-band minimum (CBM) of four $GaInP_2$ polytypes: $\langle\infty\rangle$, $\langle 2\rangle$, $\langle 3\rangle$, and $\langle 4\rangle$ belonging to the type-a series. From these four calculated LDA values we then determine four interactions (J_0, J_2, J_4, and J_6) for each physical property. Using this calculated $\{J_{k\leqslant 6}\}$ we then predict from Eq. (1) the properties of other polytypes, not used in the fit. Table II shows the directly calculated LDA results for the $GaInP_2$ polytypes, and in parentheses, the values obtained from the Ising expansion, using the fitted $\{J_{k\leqslant 6}\}$. Figure 4 plots the band-gap energy and the VBM and CBM energies as a function of the layer thickness n of the APB superlattice $\langle n\rangle$. Similar calculations were performed for type-b polytypes $CuInSe_2$ (Table III). We note the following observations.

(i) *Formation energies*. The Ising expansion converges rapidly for the formation energies. Within the accuracy of the underlying LAPW calculation, one needs to retain only J_2 and J_4 for the $GaInP_2$ polytypes. For the $CuInSe_2$ polytypes, only J_2

little effect on their electrical and optical properties. In contrast, $E_g(\mathrm{CH})\ 2\ E_g(\mathrm{CuAu})\ 5\ 232$ meV for $CuGaSe_2$. Thus, the effect is larger for $CuGaSe_2$.