E t act g *E* e $\vec{k}$ effect e ba d t ct e f e ce ca c at a a d e

Voicu Popescu[1,2,*] and Alex Zunger[3,†]

[1]*Physics Department and REMRSEC, Colorado School of Mines, Golden, Colorado 80401, USA*

[2]*National Renewable Energy Laboratory, Golden, Colorado 80401, USA*

[3]*University of Colorado, Boulder, Colorado 80302, USA*

(Received 21 October 2011; published 2 February 2012)

The supercell approach to defects and alloys has circumvented the limitations of those methods that insist on using artificially high symmetry, yet this step usually comes at the cost of abandoning the language of E versus $\vec{k}$ band dispersion. Here we describe a computational method that maps the energy eigenvalues obtained from

III. CONSTRUCTING THE EFFECTIVE BAND STRUCTURE OF A RANDOM ALLOY

We describe in this section the actual construction of an EBS for an alloy, using the specific example of $In_{0.1}Ga_{0.9}N$, a system that preserves, to a large extent, a recognizable band structure ("a weakly perturbed alloy").[6] The necessary steps for an alloy EBS determination—illustrated in Fig. 2—are the following:

(A) Choosing the SC to be used in modeling the alloy system, deciding on a reference PC and a set of wave vectors $\{\vec{k}_i\}$ over which to construct the EBS. As we discuss in more detail below, this set needs to be extended to include also the additional PC wave vectors that are equivalent by symmetry with $\vec{k}_i$. We denote this extended set by $\{\vec{k}_j\}$;

(B) Decorating the SC, one random realization at a time;

(C) Relaxing the atomic positions so as to minimize the elastic energy;

(D) Calculating the SC eigenvalues and eigenvectors;

(E) Determining the set $\{A(\vec{k}_j, E)\}$ of SFs for all $\vec{k}_j$ vectors of step (A), and calculating an internal average over those $\vec{k}$ vectors that are equivalent by symmetry with $\vec{k}_i$, which provides a subset of *averaged*, representative SFs $\{\bar{A}(\vec{k}_i, E)\}$; and

(F) Repeating steps (B)–(E) if different random realizations are used. The statistically averaged SFs at each $\vec{k}_i$ are collected into the EBS. This final product (a typical EBS) is shown in Fig. 2(b) and will serve as a general template for the rest of the results presented in this paper.

A. I a et g : The e ce , the efe e ce a d the et f e wa e ect

1. Setting up the supercell

A

3. The extended set of primitive and supercell wave vectors

Let us assume that we have decided to construct the alloy EBS for a set $\{\vec{k}_i\}$ of a chosen pbz. We enforce the *macroscopic*

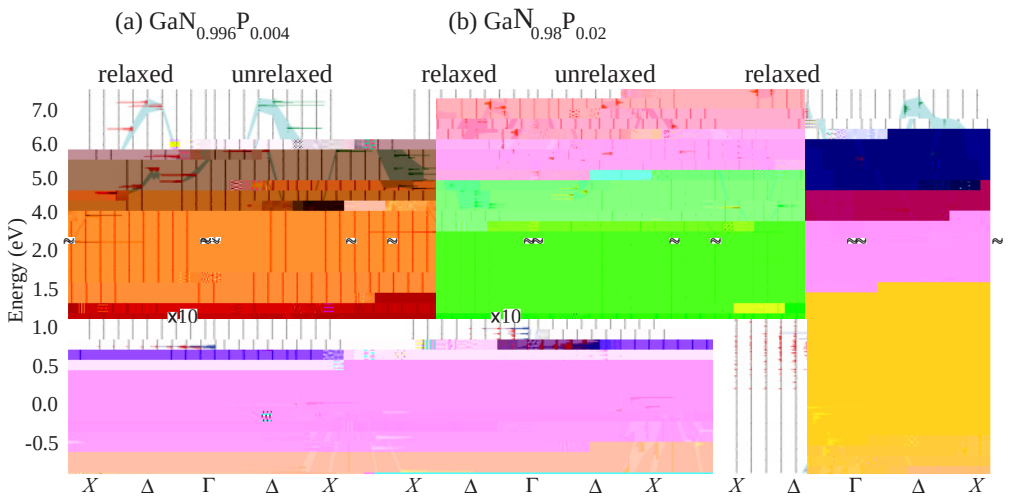
in the EBS construction and discussion is the cumulative sum,[20]

$$S_{\vec{k}_i}(\mathcal{E}_n) = \int^{\mathcal{E}_n} \bar{A}(\vec{k}_i, E)dE, \tag{17}$$

depicted in the same panels as $\bar{A}(\vec{k}_i, E)$ with blue (black) lines. This cumulative sum is characterized by steps of value $g(\vec{k}_i)$ whenever an "alloy band" of degeneracy $g(\vec{k}_i$

have performed calculations for all possible n_c values between the two limits—total randomness ($n_c = 1$) and complete clustering ($n_c = n_{\max}$)—we show only two illustrative cases, in which the P clusters are of intermediate size $1 < n_c \leqslant n_{\max}$. Here we should note that, when modeling a disordered $A_{1-x}B_x$ system within a SC approach the composition x takes on only discrete values, rather than being a continuous variable.

The general trend to be observed when moving from perfect disorder ($n_c = 1$) to complete clustering ($n_c = n_{\max}$) is the


(a) GaN0.996P0.004
(b) GaN0.98P0.02
relaxed
unrelaxed
relaxed
unrelaxed
relaxed
Energy (eV)
7.0
6.0
5.0
4.0
2.0
1.5
1.0
0.5
0.0
-0.5
x10
x10
X Δ Γ Δ X X Δ Γ Δ X X Δ Γ Δ X

We assume the PC eigenvectors $|\vec{k}_0 n\rangle$ to be of an analogous form

$$|\vec{k}_0 n\rangle = u_{\vec{k}_0 n}(\vec{r})\, e^{i\vec{k}_0\vec{r}} = \left[\sum_{\vec{g}} B_{\vec{k}_0 n}(\vec{g})\, e^{i\vec{g}\vec{r}}\right] e^{i\vec{k}_0\vec{r}} \quad \vec{k}_0 \in \text{pbz}, \tag{A2}$$

and satisfying the orthogonality condition [Eq. (11)]. We note that the distinction between the two mappings, SBZ and pbz, of the reciprocal space is directly reflected in the two different summations over $\vec{G}$ and $\vec{g}$ in Eqs. (14) and (A2). From Eq. (11), using the ansatz (A2) one obtains the following:

$$\begin{aligned}\delta_{nn'} &= \langle \vec{k}_0 n|\vec{k}_0 n'\rangle \\ &= \sum_{\vec{g},\vec{g}'} B^{*}_{\vec{k}_0 n}(\vec{g})\, B_{\vec{k}_0 n'}(\vec{g}')\int d^3 r\, e^{i(\vec{g}'-\vec{g})\vec{r}} \\ &= \sum_{\vec{g}} B^{*}_{\vec{k}_0 n}(\vec{g})\, B_{\vec{k}_0 n'}(\vec{g}),\end{aligned}$$

or

$$\sum_{\vec{g}} B^{*}_{\vec{k}_0 n}(\vec{g})\, B_{\vec{k}_0 n'}(\vec{g}) = \delta_{nn'}. \tag{A3}$$

One can look upon the expansion coefficients $B_{\vec{k}_0 n}(\vec{g})$ as elements of a matrix $\underline{\widetilde{B}}$, with $\widetilde{B}_{n\vec{g}} = B_{\vec{k}_0}$