INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

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CALCULATED USING THE RECURSION METHOD

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THE ELECTRONIC STRUCTURE OF Ga As$_{1-x}$P$_x$ AND Ga Sb$_{1-x}$P$_x$
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ABSTRACT

The electronic structure calculation of Ga As$_{1-x}$P$_x$ and
Ga Sb$_{1-x}$P$_x$ alloys using the recursion method is reported.   A five
orbitals, sp^{3}s*, per atom model is used in the tight-binding
representation of the Hamiltonian.

The local density of states are calculated for Ga, As, Sb
and P-sites, in a cluster of 216 atoms, the results are reasonably
in good agreement with previous calculations.

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I. INTRODUCTION

There have been extensive experimental studies of the
electronic structure of ternary alloys because of their impor-
tance in optoelectronic device applications.[1-5]   A quantitative
understanding of the main features of the electronic band struc-
ture such as the compositional variations of band gaps, has been
obtained. The theoretical work, on the other hand, has not been
extensive mainly due to the difficulty in handling the disorder
effects.

The virtual-crystal (VCA) and coherent-potential (CPA)
approximations are used to study Ga AS$_{1-x}$P$_x$ alloys[6-9]. Chen and
Sher[6], in their CPA calculations found almost no difference from
the VCA results. There is a very small difference only in the
lower part of the conduction bands in their Figure 4 for
Ga As$_{0.5}$P$_{0.5}$. This may mean that the effect of alloy scattering is
not significant. There is an indirect-to-direct-gap   crossover for
P concentration experimentally measured to be x_c=0.45[10]   (77 K)
and x_c=0.51[11]   (30 K). The experimental situation for the L$_1$ gap is
uncertain.

The alloy disorder effects is argued to be important for
Ga Sb$_{1-x}$P$_x$ alloy due to the large differences in the s- and p-
orbital atomic energies of P and Sb[9]. Apparently, there is no
experimental data available for this alloy to compare with.

In this work, we apply the recursion method to study the
electronic properties of Ga AS$_{1-x}$P$_x$ and Ga Sb$_{1-x}$P$_x$ alloys. The
paper is organized in the following manner. A brief summary of
the most important aspects of the recursion method is given in
section II. The details of the calculation and the results are
summarized in Section III.

II. THE RECURSION METHOD

The recursion method is amply discussed in the literature
Therefore   only   a brief discussion of the essentials is given [12].
here, the main quantity of interest in the recursion method is the
local density of states (LDOS) which is defined by

$$N_\alpha(E,\vec{R}) = \sum_n |<n|\alpha R>|^2 \, \delta(E-E_n), \tag{1}$$

where $|n>$ and E_n are eigenfunctions and eigenvalues of the system
and $|\alpha\vec{R}>$ is a localized orbital α located at R. Using the Green
function $G(E) = (E-H)^{-1}$, Eq. (1) can be rewritten as,

$$N(E,R) = \frac{-1}{\pi} \lim_{\delta \to 0} Im <\alpha\vec{R}|G(E+i\delta)|\alpha\vec{R}>. \tag{2}$$

The method generates by means of the following recursion algo-
rithm an orthogonal basis $|n\}$, which contains the orbital $|\alpha\vec{R}>$
as starting element $|0>$ and in which the Hamiltonian H is
tridiagonal

$$b_{n+1}|n+1> = (H-a_n)|n> + b_n|n-1>, \tag{3}$$

$$<n\,H\,m> = \begin{cases} a_n & \text{if } m = n \\ b_n & \text{if } m = n+1 \\ b_n^* & \text{if } m = n-1 \\ 0 & \text{otherwise}. \end{cases} \tag{4}$$

The 0-0 element of G

$$<0|G|0> = \cfrac{1}{E-a_0 - \cfrac{|b_1|^2}{E-a_1 \dots}} \tag{5}$$

is equal to the local density of states $N_\alpha(E,\vec{R})$. Thus, the
essential information needed for LDOS is contained in the set of
coefficients a_n, b_n. Once the coefficients a_n, b_n are determined,
the continued fraction (5) can immediately be calculated for any E.

III. RESULTS AND CONCLUSIONS

The recursion method is of course not providing detailed
k-space information about the band structure. But it yields
valuable information on LDOS at chosen atomic sites. Encouraged
with the smallness of the alloy scattering effects we use an
interpolation procedure and try to make a reliable use of known
properties of the constituent binaries GaAs, Gap and GaSb.

A cluster of 216 atoms in zincblende structure with a
lattice constant a = 5.6537 Å is used for GaAs. The Slater-Koster
(SK) parameters used in describing the Hamiltonian H are given in
Table 1. The five orbitals, sp^3s^*, per atom are used so that there
are 1080 orbitals in the system. Here s* is the extra s-orbital
introduced to correct the lower conduction bands instead of
extending the interactions to second nearest neighbors.

The same model is used to study GaP and GaSb. The cluster,
in these cases, is arranged in the zincblende structure with a
lattice constant a = 5.4505 Å and a= 5.8732 Å respectively. The SK
parameters used are given in Table 1. The number of recursion

coefficients a_n , b_n^2 calculated in all cases reported in this section is 17. we present the calculated LDOS curves for $Ga\ As_{0.5}\ P_{0.5}$ and $Ga\ Sb_{0.5}\ P_{0.5}$. Figures. 1-6 show the LDOS for Ga, P , As, and Sb-sites in the two alloys studied respectively. Although calculated, the integrated DOS and structural energies are not presented for   simplicity. The last two Figures 7 , 8 show the orbital decomposition of LDOS for Ga-site in $Ga\ As_{1-x}\ P_x$. In all calculations presented we used an averaging procedure where the interaction parameters and the lattice constant for the ternary $A_x B_{1-x} C$ are taken as

$$V_{alloy} = V_{AC} + (V_{BC} - V_{AC})(1-x)$$

$$a_{alloy} = a_{AC} + (a_{BC} - a_{AC})(1-x)$$

Self energies of the same type of atoms are also averaged so the concentration dependent of each environment is approximately taken into account. The orbital decomposition of all LDOS curves calculated is as expected. Including extra orbitals,like Ga 3d for example, may affect the lower part of the valence bands. But this would be negligible since Ga 3d levels lie about 6 eV below the 4s levels.

To study the band gap variation with P concentration is not easy within the recursion method because of the inherent difficulties with band gabs in this technique. They do not come out sharp enough for easy identification.

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Table 1. Slater Koster parameters for GaAs, GaSb and GaP (eV)

| Semicond. / Parameter	GaAs	GaSb	GaP
$-ss\sigma$	1.6133	1.5392	1.8677
$s_a p_c \sigma$	1.9399	2.1478	1.8520
$-s_c p_a \sigma$	2.5045	2.0211	2.7362
$pp\sigma$	3.0276	2.4590	3.1063
$-pp\pi$	0.7808	0.6633	0.7456
$s^*_a p_c \sigma$	2.0967	2.1605	2.0153
$-s^*_c p_a \sigma$	2.0818	1.8265	2.0266
$-E(s,c)$	2.6569	3.8993	2.1976
$-E(s,a)$	8.3431	7.3207	8.1124
$E(p,c)$	3.6686	2.9146	4.1150
$E(p,a)$	1.0414	0.8554	1.1250
$E(s^*,c)$	6.7386	5.9846	7.1850
$E(s^*,a)$	8.5194	6.6354	8.5150
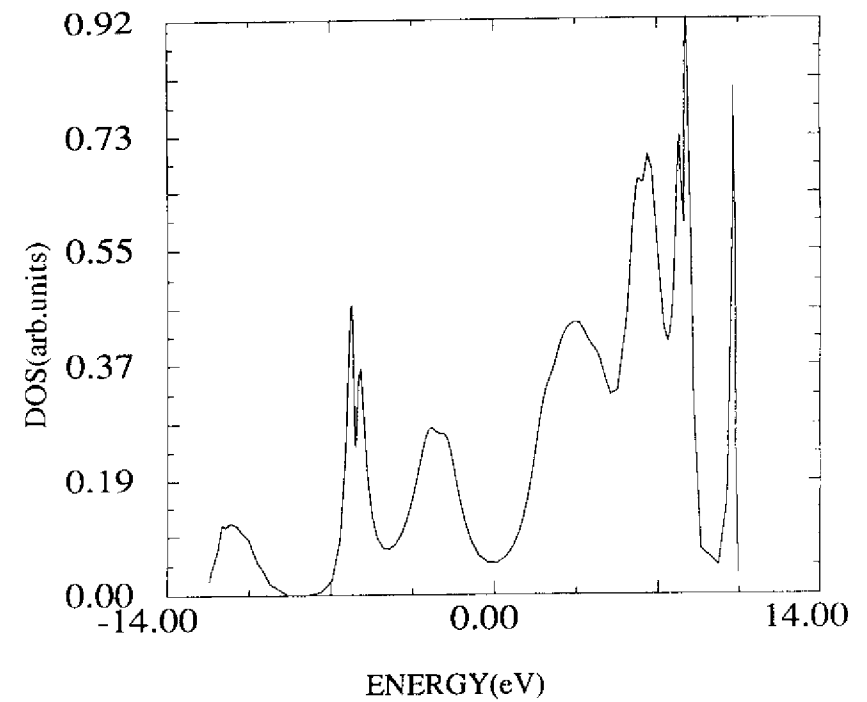
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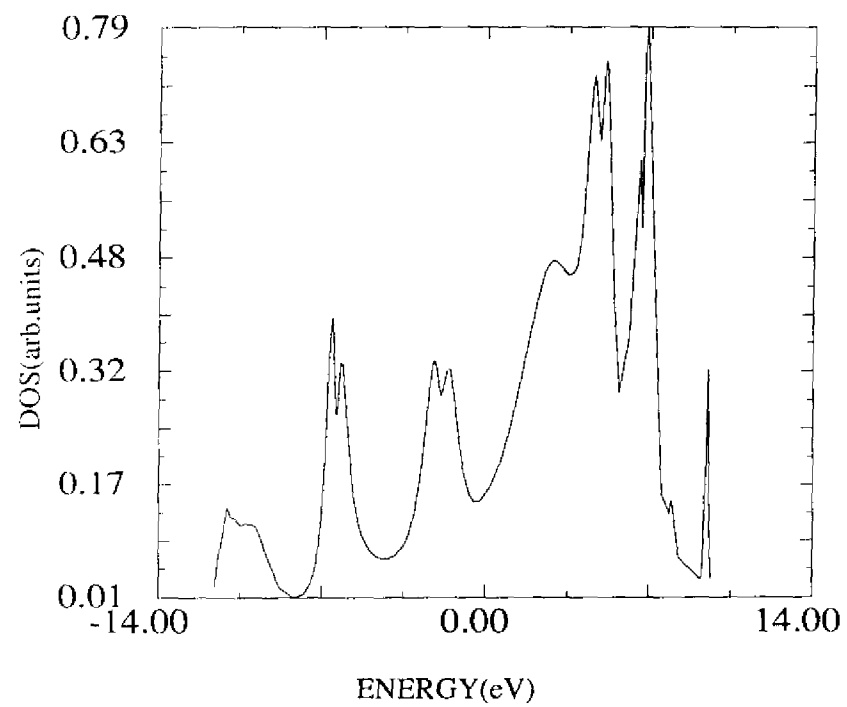
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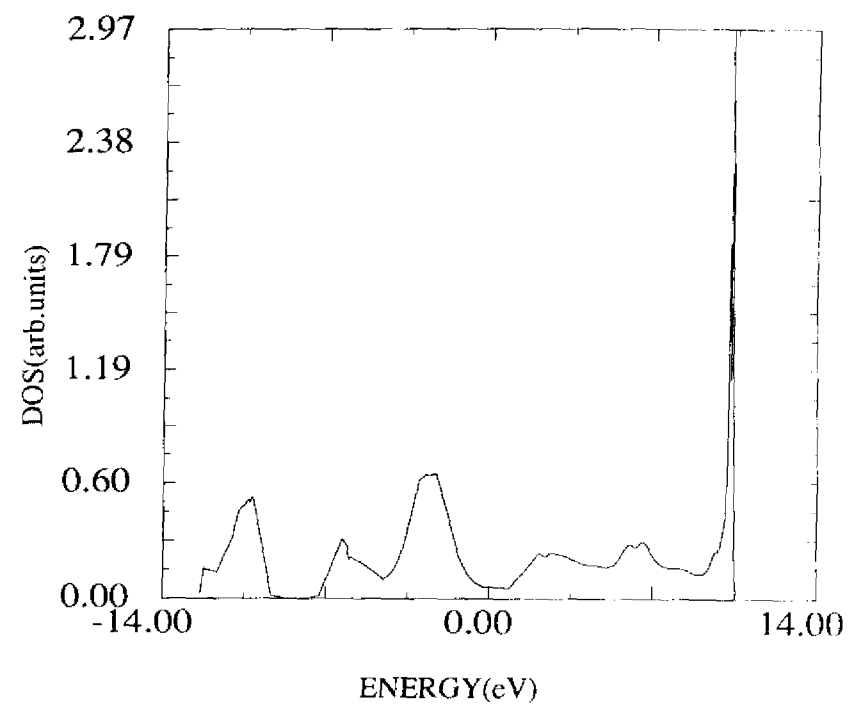
Fig.3

Fig.4

Fig.5

Fig.6

Fig.7

Fig.8