Effect of Mn concentration and strain on the band structure of GaMnAs: Theoretical study

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Abstract-Among all magnetic semiconductors, GaMnAs seems to be the most important one. In this work we present a comprehensive, accurate up to date compilation of GaMnAs band parameters at zero temperature using the k.p method based on complete and consistent parameter sets [1]. Due to the magnetic aspect of GaMnAs, we have studied the effect of manganese on the structure band by varying the Mn concentration range and the strain as well. Furthermore, we have calculated the energy gap and the heavy holes effective masses. The results show that by increasing the strain and Mn composition, the energy gap decreases which agree well with the most recent studies. [2]

I. INTRODUCTION

The ferromagnetic semiconductor GaMnAs based on GaAs, has proven to ba a promising material. It has received a considerable attention and has been studied intensely over the last two decades which has earned it to become a model system for diluted magnetic semiconductors[3-4]. The interest in these materials has been renewed due to their potential application in several fields such as spintronics devices and by dint of its structural compatibility with most epitaxially grown III-V semiconductors.Thus, they can act as a source of spin-polarized carriers in the absence of external magnetic fields. In contrast to classic semiconductors, the electronics properties of DMS are strongly influenced by many parameters. Among those material parameters, lattice strain and Mn concentration play a crucial role in varying the band structure. In this work, we theoretically studied the influence of strain and Mn composition on the electronic band structure behavior of GaMnAs.

II. COMPUTATIONAL DETAILS

From a theoretical outlook, first principles computations can provide handy information about electronic and structural properties of GaMnAs. In general terms, most of these computations are based on density functional theory (DFT) coupled to the local density approximation (LDA) or to the generalized gradient approximation (GGA) for the exchange-correlation (XC) functional [5] in which the band gap, which is a fundamental property of a semiconductor, is always underestimated in both LDA and GGA approximations. To provide complete information regarding the band gap and electronic properties, calculations have been carried out using the 8-bandk.p method due to the power of symmetry analysis that manifested itself in the non-perturbative k.p analysis of semiconductor band structure by Kohn and Luttinger [6], furthermore, it led to the development of full-zone k.p calculations such as established by [7]. In this article, the computations were performed using the 6-band Kohn – Luttingerk.p Hamiltonian for GaAs given by Dietl et al. [8], and 8-band Kane in Ostromek parameterization taking into account the inversion asymmetry of GaAs [9]. The values of Luttinger parameters employed in our calculations are depicted in **Table 1**, while the additional optimized parameters of Kane Hamiltonian are listed in **Table 2**.Moreover, in this

parametrization, the spin-orbit splitting of Γ_8 and Γ_7, Δ_{SO}, equals to 0.341 eV and the complete Hamiltonian for the wave vector k is:

$$H(k) = H_{k.p}(k) + M_{kSO} + H_{BS}(\varepsilon) + \Delta s^z$$

Where $H_{k.p}(k)$ is the k.p Hamiltonian matrix, $H_{kSO}$the matrix describing the k-dependent part of the spin-orbit interaction, $H_{BS}(\varepsilon)$is the strain operator matrix and finally s^z is spin operator matrix[1].The spin-orbit interactionis considered following Ref. [10].

Table 1. Luttinger parameters for k.pHamiltonians

Parameters	Kohn - Luttinger
γ_1^l	6.85
γ_2^l	2.10
γ_3^l	2.90

Table 2. Additional parameters of the Kane 8x8 Hamiltonian

Parameters	Values
Ev ≡ E (Γ_8) [eV]	0
Ec ≡ E (Γ_6) [eV]	1.1519
A’ [eV Å²]	-14.70
E_p[eV]	29.112
C_0[eV Å²]	0.1564
B [eV Å²]	39.11

III. RESULTS AND DISCUSSION

In the first part we will discuss the effect of strain and Mn composition on the structure band of GaMnAs. Based on our calculations carried out at 0 Kelvin, a change of the Mn composition and both tensile and compressive strain as well, would result in the change of the band structure as shown in **Figure 1**.

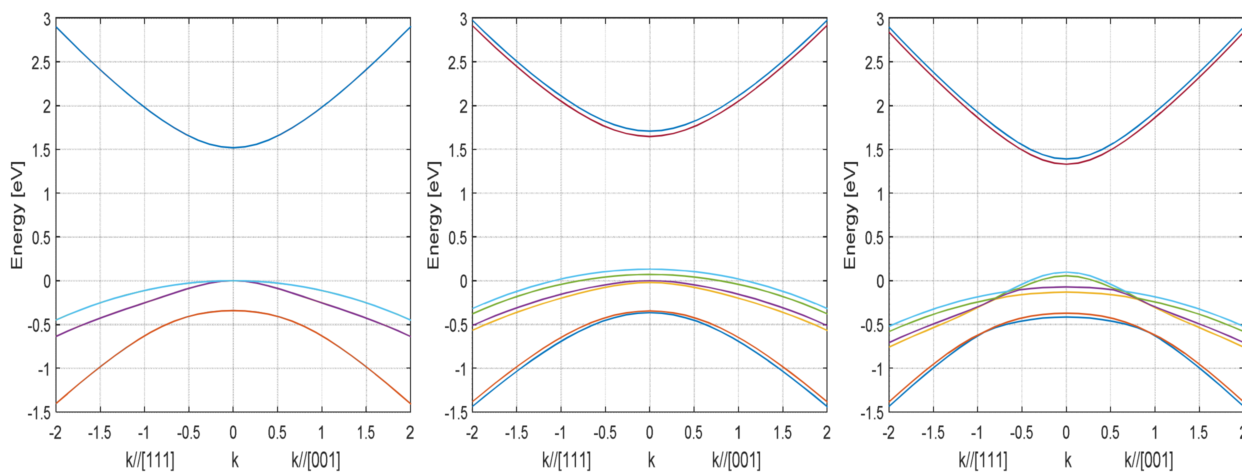

Figure 1: (a) Pure GaAs band structure, (b) GaMnAs band structure under tensile strain of -1% with Mn concentration of 1%, (c) GaMnAs band structure under a compressive strain of 1% with Mn concentration of 1%

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The figure above unveils that the strain and Mn composition yields qualitative effect on the electronic band structure by lifting the degeneracy of the light and heavy holes bands and spin-splitting of the bands induced by the sp-d exchange interaction [1].
Thus, we start our studies by calculating the energy gap while varying the strain continuously from tensile to compressive along with varying the Mn composition within the range of x=0.01 to x=0.1. For each concentration, we calculate the spin-up band gap. This precious information can be of use in the design of spintronic devices [11-12]. Now we focus our attention on the band gap dependence on the Mn content and applied strain. We consider this band gap as the energy difference between the lowest spin-up conduction band state $\Gamma_6$and the highest spin-upstate in the valence band Γ_8. In **Figure 2** we plot the results and according to them it's worth noticing that the band gap decreases by increasing the Mn amount and expanding the strain.

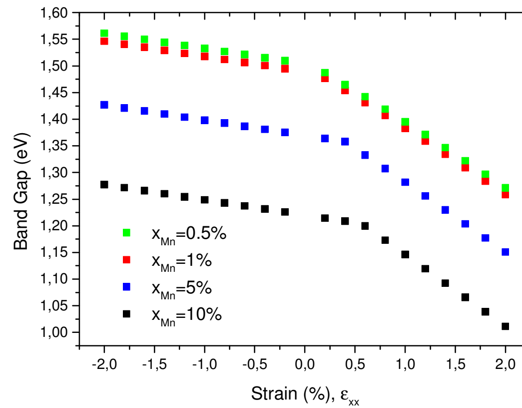

Figure 2: Energy gap as a function of the strain and Mn composition

Spin band gap of GaMnAs considering recent compilations published by Dietl et al. [8] and Thomas et al. [13], compared with our calculations show a good agreement. Besides, these findings are also endorsed by the theoretical calculations ofTureket al.[14]. To fully exploit our results, we provide analytical expressions for the energy band gap which could be of practical use and of simple access taking into account both parameters; Mn concentration and strain.

$$E_g = 1.519 - 0.0299\, x_{Mn} - 0.02866\, \varepsilon_{xx}$$: Energy band gap for tensile strain

$$E_g = 1.519 - 0.0299\, x_{Mn} - 0.01275\, \varepsilon_{xx}$$: Energy band gap for compressive strain

However, the expressions we came out with, combining the strain and the Mn composition, seem to be established for the first time according to the literature.As a complement to the band gap, which is the main focus of this work, we also provide an overview of heavy holes (HH) effective masses computations.We show in **Figure 3** the HH effective masses as a function of strain and Mn composition. The HH effective masses are found to increase by the strain ranging from -1% (tensile strain) to 2% (compressive strain) and by increasing the Mn amount from 1% to 7% all along [001] which is parallel to the aimantation axis. However, as shown in **Figure 4,** along [100] which is perpendicular to the aimantation axis, the HH effective masses seem to be decreasing by varying the strain from tensile to compression and by increasing the Mn composition as well. This behavior is the opposite of the one observed along [001] due to the symmetry of the crystallographic directions.

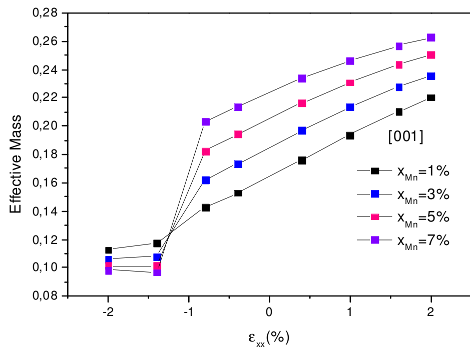

Figure 3: HH effective masses as a function of the strain and Mn composition along [001]

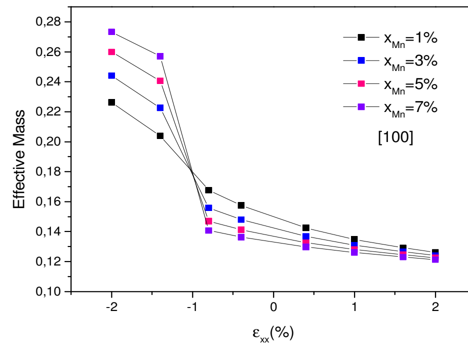

Figure 4: HH effective masses as a function of the strain and Mn composition along [100]

Furthermore, in **Figure 5** and **6**, computations carried along [110] and [111] depict that HH effective masses variation is similar to the variation observed along [100].

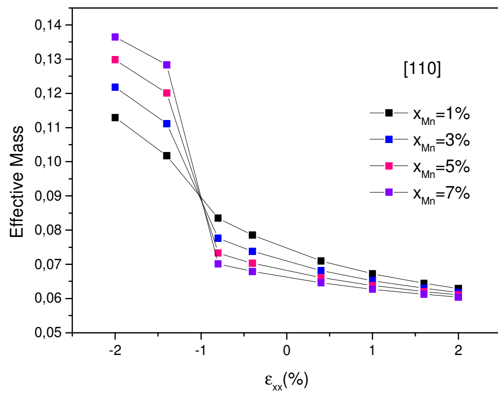

Figure 5: HH effective masses as a function of the strain and Mn composition along [110]

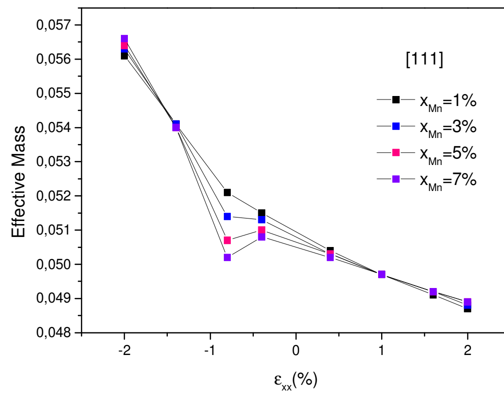

Figure 6: HH effective masses as a function of the strain and Mn composition along [111]

In addition, we calculated the HH effective masses for each concentration; 1%, 3%, 5% and 7%, as function of the strain and the crystallographic direction. The figures below indicate that along [100], [110] and [111] the HH effective masses decreases by increasing the strain due to the flattening of bands, while, when it comes to the calculations carried along [001] the HH effective masses seem to be increasing. We suggest that the fact that aimantation axis is parallel to [001] is behind the increase of HH effective masses which still to be proven experimentally.

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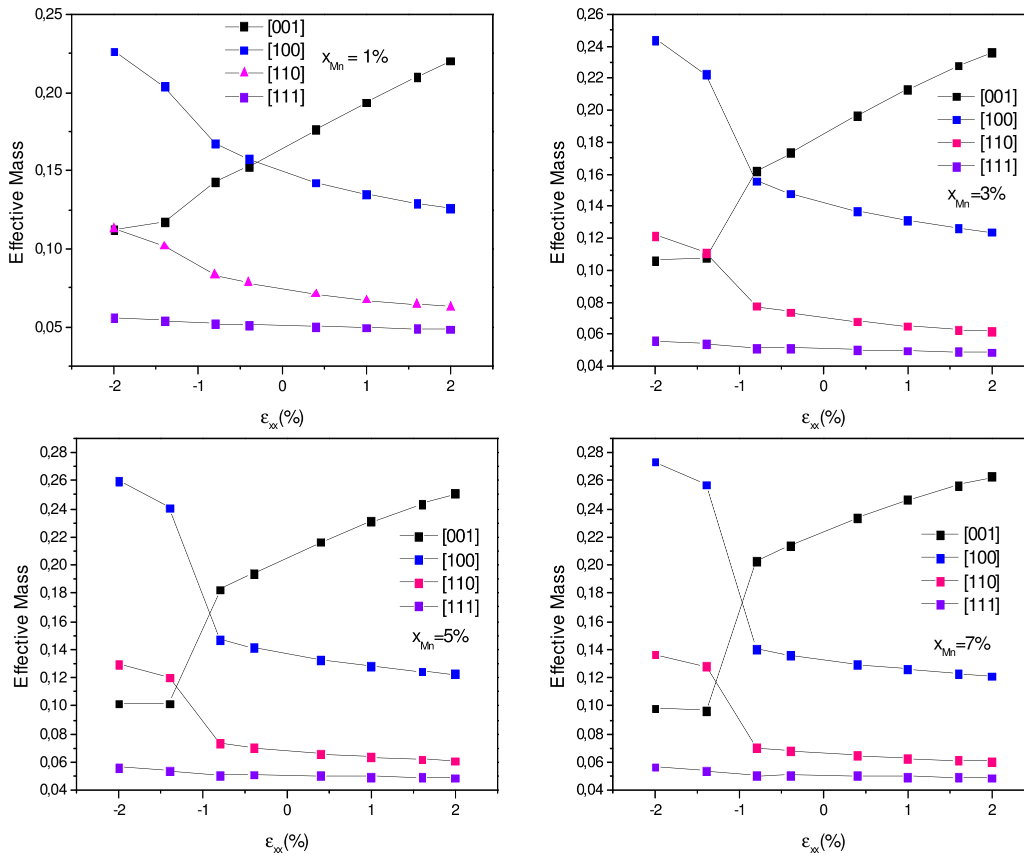

Figure 7: HH effective masses as a function of the strain and the crystallographic direction

IV. CONCLUSION

In summary,we have studied theoretically the GaMnAsmagnetic semiconductor (MS) within the 8-bandk.pmethod and we calculated the band gap while varying Mn concentrations and strain from tensile to compressive.We obtained a good agreement between our results and the most computational methods reported for this material.From the calculated energy gap, we derived practical and of simple access expressions for Eg combining for the first time both Mn concentrations and strain for this magnetic semiconductor which is the main striking achievement in this work. These calculations, in addition to other ones done before, show that the 8-bandk.p technique can indeed be used to estimate accurately the energy gap, opening a window to explore other relevant MSs such as GaMnN, InMnN, InMnAs, etc.Due to our theoretical model, we have been able to reproduce correctly the HH effective masses at the center of the BZ ensuring that the curvature of the energy bands is accurately reproduced.

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