 

# Growth and characterization of $Ge_{1-x}Sn_x$ alloys grown by magnetron sputter deposition

H. Pérez Ladrón de Guevara, H. Navarro-Contreras, M.A. Vidal
*Instituto de Investigación en Comunicación Óptica (IICO), Universidad Autónoma de San Luis Potosí (UASLP),S.L.P., Avenida Karakorum 1470, Lomas 4ta sección,CP 78210, San Luis Potosí, S.L.P.,Mex.*

Single phase $Ge_{1-x}Sn_x$ alloys have been grown on Ge(100) and GaAs(100) substrates using a R. F. Sputtering system. Using HRXRD on asymmetrical planes in plane and in growth lattice parameters are obtained. A residual strain due to the differences in the linear thermal expansion coefficient between the alloy and the substrates is observed.

***Keywords:*** $Ge_{1-x}Sn_x$ alloys; HRXRD; Sputtering deposition

## 1. Introduction

One of the most fascinating ideas of the semiconductors physics is the realization of a direct band gap material based fully on group IV elements. The metastable $Ge_{1-x}Sn_x$ alloy has the potential of a tuneable direct energy gap material with Sn composition. It had been probed that a direct band gap transition prevails for Sn concentrations below 0.15, with direct band gap transition between 0.35 and 0.79 eV [1-2] [Fig 1]. Furthermore, very low effective electron masses are predicted for the alloy and hence high electron mobility[3-5].

The growth of this alloy is very difficult due to the lattice mismatch (14.7 %). The solid solubility limit of Ge in diamond structure Sn is 1% and Sn tends to segregate to the surface. Bulk Sn transforms from α-phase (diamond cubic, gray tin) to β-phase (body-centred tetragonal, white tin) at $13.2^0$C[6-8] . But in non equilibrium growth systems like MBE or Sputter Deposition it is possible to grown these alloys at temperatures between 100 and $200^0$C[1,3,4].

## 2. Experimental Procedure

In a RF sputtering system were grown single phase $Ge_{1-x}Sn_x$ alloys with Sn concentrations $0<x<0.14$ on Ge(100) and GaAs(100) substrates. Varying growth parameters such as growth temperature, pressure in the chamber and the power of the targets of Ge and Sn. Sn concentration of the alloy were calculated from the bulk lattice constant of the film using High Resolution X-Ray Diffraction (HRXRD) of the Rocking Curves (RC) on the asymmetrical planes (115) and (-1-15).

## 3. Experimental Results

Using the angular separation between the diffraction substrate signal and the diffraction signal of the film on the asymmetric planes [Figs. 2 and 3], lattice constants of the alloy are obtained [9]. We assume a linear dependence of the lattice constants (Vegard's Law) and elastic constants of the alloy. Sn concentration of the alloy is determined by the bulk lattice parameter calculated from the in-plane and in growth lattice parameters.

The results obtained by HRXRD analysis indicate that the films grown on Ge(100) and GaAs(100) are pseudomorphical in the composition range $0<x<0.04$ since the in-plane lattice parameters of the $Ge_{1-x}Sn_x$ alloys have the same value of the substrate lattice parameter as is shown in figure 4. In the composition range $0.04<x<0.10$ the in plane and in growth lattice parameters are closing to the alloy bulk parameter. In the films grown o n Ge(100) the films are fully relaxed at Sn concentrations $x>0.10$. But this fact is not observed for the films grown on GaAs(100) substrates.

Any strain due to differences in the linear thermal expansion coefficient (LTEC) between $Ge_{1-x}Sn_x$ and Ge is not observed under the experimental conditions reported. We estimate that the deformation expected to this difference thermal expansion is $\varepsilon_{||} = 2x10^{-6}$ for the case of x = 0.14. This behaviour is produced not only because the LTEC of the alloys and Ge substrate are very close, but also because the LTEC of the alloy crosses the LTEC of Ge around 355 K (~80 $^O$C). As can be seen in Figure 5, both the LTEC of the alloy and substrate counterbalance to produce $\varepsilon_{||}=0$ ($\varepsilon = \int(\alpha_{alloy} - \alpha_{substrate})dT$ ). However, in the case of $Ge_{1-x}Sn_x$/Ge/GaAs(100) the strain due to differences in the LTEC between the alloy with x = 0.14 and GaAs substrate is $\varepsilon_{||}$ = 1.5 X $10^{-3}$. This strain produces a difference between $a_\perp$ and $a_{||}$ that is consistent with the data observed for all Sn concentrations in Figure 4.

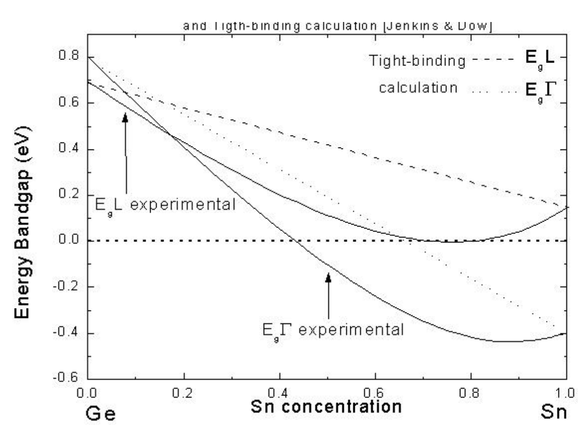


**Figure 1.** Predicted band gap structure by Thigh-binding calculations and experimentally measured band gap for $Ge_{1-x}Sn_x$ alloys.

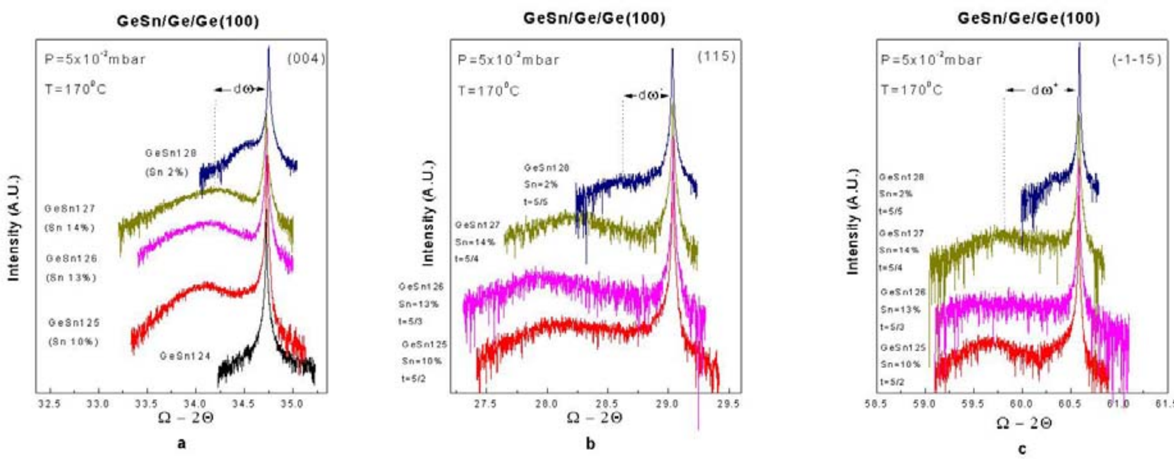


**Figure 2.** Rocking curves obtained by HRXRD on the **a)** (004), **b)** (115) and **c)** (-1-15) planes for the $Ge_{1-x}Sn_x$/Ge/Ge(100) heteroestructures.

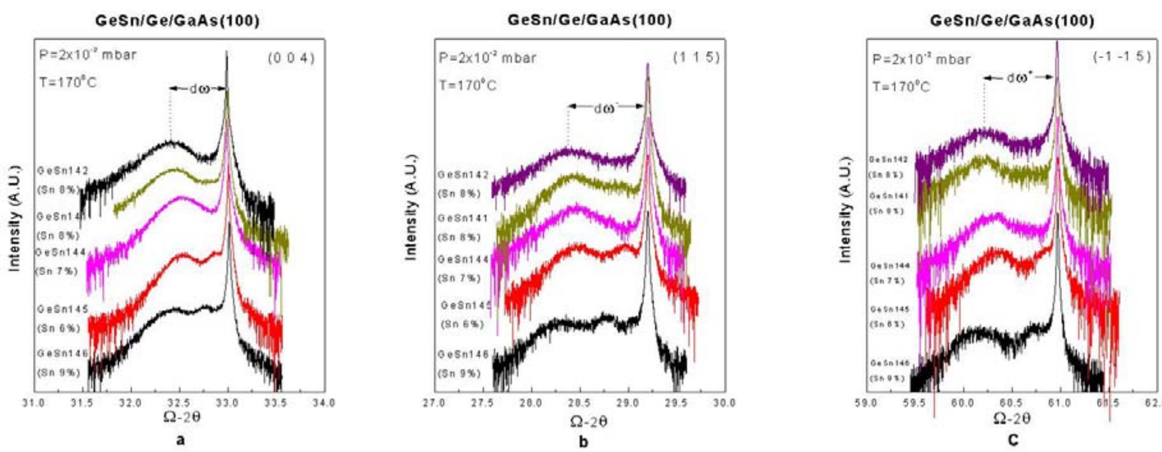


**Figure 3.** Rocking curves obtained by HRXRD on the **a)** (004), **b)** (115) and **c)** (-1-15) planes for the $Ge_{1-x}Sn_x$/Ge/GaAs(100) heteroestructures.

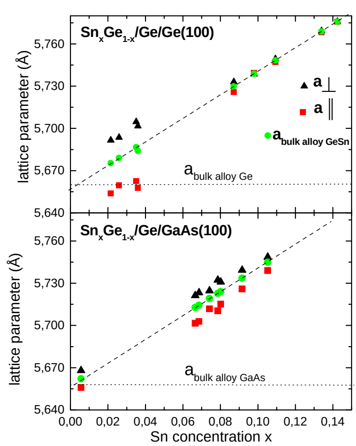


**Figure 4.** The $a_\perp$ (in-growth), $a_{||}$ (in-plane) and $a_0$ (bulk) lattice parameters are shown as function of Sn concentration.

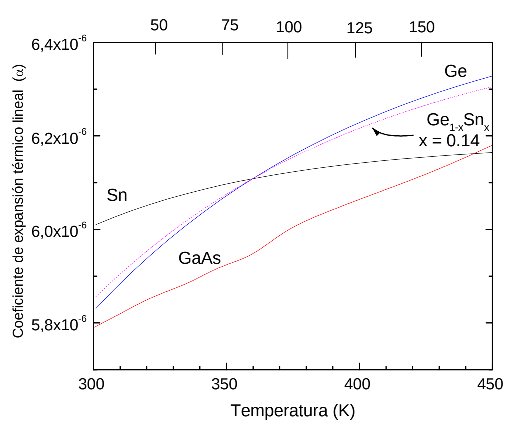


**Figure 5.** Linear thermal expansion coefficient of Ge, GaAs, Sn and $Ge_{0.86}Sn_{0.14}$

## 4. Conclusions

Single phase $Ge_{1-x}Sn_x$, alloy films have been grown on Ge(100) and GaAs(100) substrates with Sn concentration up to 14% according HRXRD measurements. The films are pseudomorphical for Sn concentrations $0<x<0.04$. The films grown on Ge(100) do not show residual strain due to the differences in the LTEC.

In the future an optical characterization of the alloys will be made for the determination of the direct energy band gap and to determinate if the change of the gap is proportional to the Sn concentration of the alloy. Also a Raman analysis will be done.

## References

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