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Features of a new 3D abacus as a tool for phothovoltaic-thermal binary and ternary semiconductor materials scaling

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ABSTRACT

In this study, a multiple physical parameters abacus is commented. The main purpose of this abacus is to optimize and evaluate photovoltaic-thermal semiconductor synthetical compounds materials efficiency.

INTRODUCTION

This study presents a new 3D abacus for scaling binary an ternary semi conductors layered materials. This abacus gathers originally three relevant and determinant parameters in the choice of oxides, sulfured compounds and similar PVC semiconductors constituants:

- The electronic bangap E_g.
- The Vickers Microhardness *Hv*.
- The Amlouk-Boubaker Optothermal Expansivity ψ_{AB}.

The latter parameter ψ_{AB}, has beeen defined in precedent published studies as the ratio of the thermal diffusivity to the optical effective absorptivity.

In the last three decades, choice of semiconductor materials for PVC buffer or windows layers was generally and sometimes soley based on the bandgap range requirements. This feature was legitimous and appropriate until appearance of new generation PV-T cells and light-heat converter devices. Actually, and due to environment and economical constraints, the thermal performance as well as the mechanic resistance are more and more taken into account.

THE 3D ABACUS FEATURES

History

In our laboratory, we tried since 1985, to produce binary and ternary compounds for light conversion purpose. In the earliest attempts, zinc-doped In_2S_3 (namely $ZnIn_2S_4$), selenized ZnS (namely $ZnS_{1-x}Se_x \mid_{0\leq x<0.5}$) and binary oxides (ZnO, TiO_2, WO_3...) have been synthesized using several processes. It was noticed that parallel to the expected enhancement in terms of bandgap shift, many other structural and morphological changes occurred.

In the same context, the recent experiment on lightly Ytterbium-doped ZnO thin films, and pure ZnO layer prepared at different substrate temparetures, exhibited

drasticall changes in physix parametaes more tha in optical characteristic.

Additional investigations yielded spectacular results about thermal an mechanical changes during elaboration process.

The electronic bangap E_g

The electronic bandgap is the common and initial choice-relevant parameter in binary and ternary semiconductors technology. It is commonly defined as the energy range where no electron states exist. It is also defined as the energy difference between the top of the valence band and the bottom of the conduction band in semiconductors. It is generally evaluated by the amount of energy required to free an outer shell electron the manner it becomes a mobile charge carrier. Since the band gap of a given material determines what portion of the solar spectrum it absorbs, it is important to choose the appropriate compound matching the incident energy range.

The choice of appropriated materials on the single basis of the electronic bandgap is becoming controversial due the narrow efficient solar spectrum width[5,35] eV, along with new thermal and mechanical requirements.

In our study, and for each material, the band gap has been calculated using measurements of the absorption coefficient α, which is related to the incident photon energy $h\nu$ by the relation:

$$\sqrt[n]{\alpha h\nu} = k \times (h\nu - E_g) \quad (1)$$

where E_g is the band gap, k is a constant ν is the frequency, h is Planck constant and n is the index indicating the transition type.

Measurements of the ν-dependent absorption coefficient α using transmittance-reflectance ($T(\lambda)$-$R(\lambda)$) spectra yielded curves of $\sqrt[n]{\alpha h\nu}\Big|_{n=2}$ versus $h\nu$. Slopes of these curves were accurate guides to determine bandgap energies *Eg*.

The Vickers microhardness Hv

The Vickers Microhardness *Hv* is a characteristic of a solid material expressing its resistance to both permanent deformation and outer material penetration. It has been demonstrated, for semiconductors layered materials, that indentation hardness correlates linearly with tensile strength. This feature is important when such structures are jointed to devices working under strong mechanical solicitations (shocks, stretching, etc.).

Figure 1 : Vickers test disposal

The mechanical measurements have been carried out using a Vickers diamond pyramidal indenter (Figure 1). The apparatus was a common Vickers test disposal.

The Amlouk-Boubaker optothermal expansivity Ψ_{AB}

The Amlouk-Boubaker optothermal expansivity is defined by:

$$\Psi_{AB} = D/\hat{\alpha} \quad (2)$$

Where D is the thermal diffusivity and $\hat{\alpha}$ is the effective absorptivity.

The effective absorptivity $\hat{\alpha}$ is defined as the mean normalized absorbance weighted by $\mathbf{I}(\tilde{\lambda})_{AM1.5}$, the solar standard irradiance, with $\tilde{\lambda}$: the normalised solar spectrum wavelength:

$$\begin{cases} \tilde{\lambda} = \dfrac{\lambda - \lambda_{min}}{\lambda_{max} - \lambda_{min}} \\ \lambda_{min} = 200.0\ nm\ ; \lambda_{max} = 1800.0\ nm. \end{cases} \quad (3)$$

and :

$$\hat{\alpha} = \frac{\int_0^1 \mathbf{I}(\tilde{\lambda})_{AM1.5} \times \alpha(\tilde{\lambda}) d\tilde{\lambda}}{\int_0^1 \mathbf{I}(\tilde{\lambda})_{AM1.5} d\tilde{\lambda}} \quad (4)$$

where: $\mathbf{I}(\tilde{\lambda})_{AM1.5}$ is the Reference Solar Spectral Irradiance.

The normalized absorbance spectrum $\alpha(\tilde{\lambda})$ is deduced from the BPES. According to this protocol, a

set of m experimental measured values of the transmittance-reflectance vector: $\left(T_i(\tilde{\lambda}_i);R_i(\tilde{\lambda}_i)\right)\Big|_{i=1..m}$ versus the normalized wavelength $\tilde{\lambda}_i\Big|_{i=1..m}$ is established. Then the system (5) is set:

$$\begin{cases} R(\tilde{\lambda}) = \left[\dfrac{1}{2N_0}\sum_{n=1}^{N_0}\xi_n \times B_{4n}(\tilde{\lambda}\times\beta_n)\right] \\ T(\tilde{\lambda}) = \left[\dfrac{1}{2N_0}\sum_{n=1}^{N_0}\xi_n' \times B_{4n}(\tilde{\lambda}\times\beta_n)\right] \end{cases} \quad (6)$$

where β_n are the 4n-Boubaker polynomials B_{4n} minimal positive roots, N_0 is a given integer and ξ_n and ξ_n' are coefficients determined through Boubaker Polynomials Expansion Scheme BPES.

Finally, the normalized absorbance spectrum $\alpha(\tilde{\lambda})$ is calculated using the relation (7):

$$\alpha(\tilde{\lambda}) = \frac{1}{d\sqrt{2}}\sqrt{\left(\ln\frac{1-R(\tilde{\lambda})}{T(\tilde{\lambda})}\right)^2+\left(\ln\frac{(1-R(\tilde{\lambda}))^2}{T(\tilde{\lambda})}\right)^2} \quad (7)$$

where d is the layer thickness.

The effective absorptivity $\hat{\alpha}$ is calculated using (Eq. 4) and (Eq. 7).

The Amlouk-Boubaker optothermal expansivity unit is m^3s^{-1}. This parameter hance can be considered either as the total volume that contains a fixed amount of heat per unit time, or a 3D expansion velocity of the transmitted heat inside the material.

THE 3D ABACUS

According to the definitions presented in §2, it was obvious that any judicious material choice must take into account simultaneously and conjointly the three defined parameters.

Consequently, it was appropriate to gather all the ohysical-related results in a global scaling tool as a guide to material performance evaluation. This tool is the new 3D abacus (Figure 2) which has been established with respect to bangap E_g, Vickers Microhardness Hv and The Optothermal Expansivity ψ_{AB}.

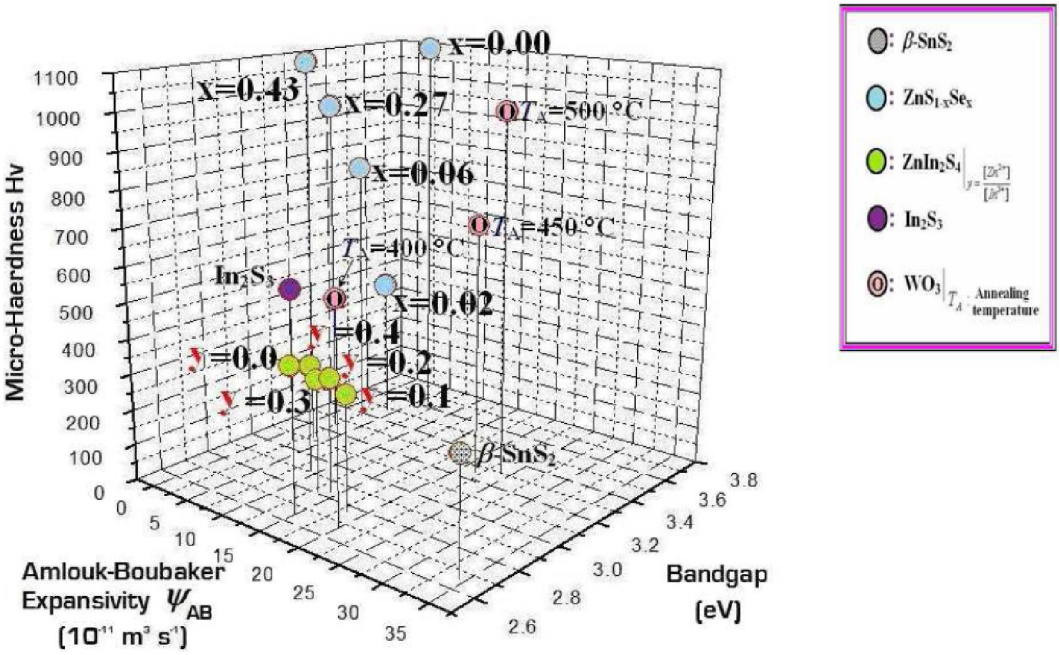

Figure 2 : 3D E_g-ψ_{AB}-Hv abacus

THE DEGENERATED 2D PROJECTIONS

For particular applications, we had to ignore one of the three physical parameters gathered in the abacus. The following 2D projections have been exploited:

Projection in Hv-E_g plane

This projection is interesting in the case of a thermally neutral material.

It is the cas, i.e. of the $ZnS_{1-x}Se_x$ compounds, it is obvious that the consideration of Bangap-Haredness features is mor important than themal proprieties. The

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E_g-*Hv* projection (Figure 3) gives a relevant information: the selenization process causes drastical loss of harndness in initially hard binary Zn-S matrial.

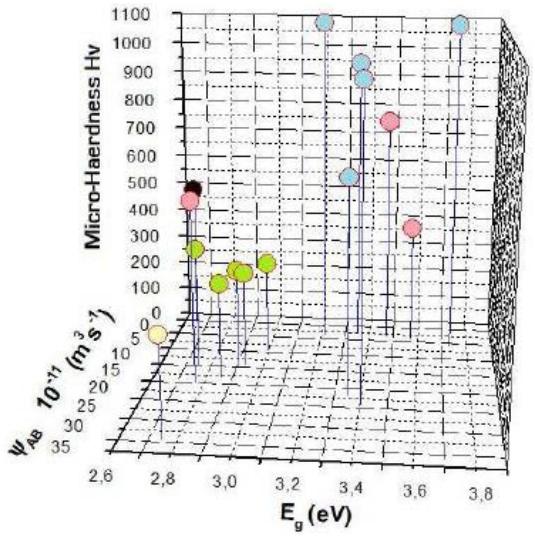

Figure 3 : E_g-*Hv* projection

Projection in ψ_{AB}-E_g plane

This projection is suitable for thick layers whose mechanical properties don't contribute significantly to the whole disposal hardness.

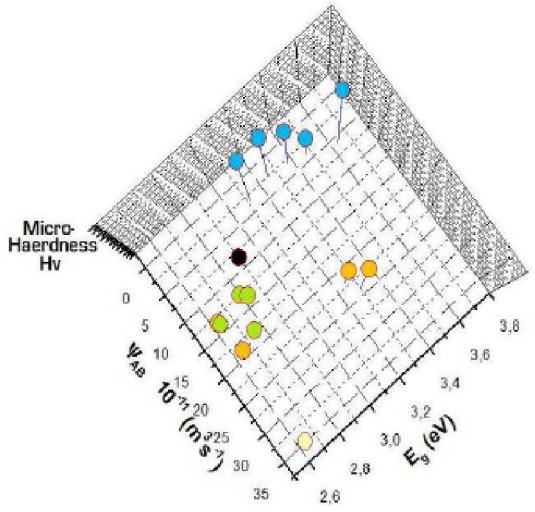

Figure 4 : ψ_{AB}-E_g projection

Projection in ψ_{AB}-Hv plane

This projection is useful for distinguishing resistant and good heat conductor materials, which is the case of the $ZnIn_2S_4$ materials.

In fact the effect of the Zinc-to-Indium ratio on the values of the Amlouk-Boubaker optothermal expansivity (Figure 5) is easily observable in this projection (it is equivalent to an expansion of the values of the parameter ψ_{AB} into a wide range:[10-19] 10^{-11} m^3s^{-1}).

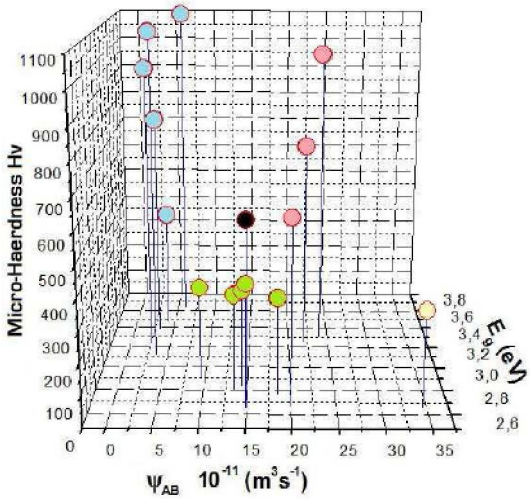

Figure 5: ψ_{AB}- *Hv* projection

CONCLUSION

This study presents the main features of a 3D abacus based on three physical parameters : the electronic bangap E_g; the Vickers Microhardness *Hv* and the lastly established Amlouk-Boubaker Optothermal Expansivity ψ_{AB}.

The usefulness of this abacus in evaluation of nanotechnology and Microelectronics-related semiconductors performance, as well as the particularities of the different projections has been presebted and discussed.

Actually, ZnO doped materials are being considered for inclusion in this evoked the existence of an optimal value for the doping mounting substrate temperature. If determined thanks to the abacus, this value will be an efficient guide to elaborating ZnO minimum-heat-continence layers.

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