Influence of Elastic Properties of Thin Films deposited on Si and/or Mg substrates on Rayleigh velocity dispersion evolution

I. Touati, Z. Hadjoub, L. Touati-Tilba, A. Doghmane*

Laboratoire des Semi-conducteurs, Département de Physique, Faculté des Sciences, Université Badji-Mokhtar, BP 12, Annaba, DZ-23000, Algérie

Received 1 January 2009; received in revised form 31 July 2009; accepted 31 August 2009

Abstract

In this work, we present a quantitative investigation of dispersion curves of Rayleigh velocity, \( V_R \), in several loading layers/(Si, Mg) substrates. For every layer/substrate system, it is shown that as the thickness, \( h \), increases the curves decrease with different slopes then saturate at variable transition normalized thickness, \( (h/\rho \gamma T_L)_0 \). To quantify the transition phenomenon, we introduced a parameter, \( \chi \), depending on \( V_R \) and densities, \( \rho \), of both layers and substrates. Hence, it was possible to deduce analytical expressions of the form: \( (h/\rho \gamma T_L)_0 = 1.16 + 0.16 \chi \) for layers/Si systems and \( (h/\rho \gamma T_L)_0 = 0.37 + 0.65 \chi \) for layers/Mg combinations.

© 2009 Elsevier B.V. Open access under CC BY-NC-ND license.

PACS: 43.35.Ae; 43.35.Ns; 43.35.Pt; 62.30.+d; 68.60.Bs

Keywords: Elastic constants; thin films; velocity dispersion; loading effect; Si; Mg

1. Introduction

Ultrasonic nondestructive characterization is based on the interaction of elastic waves with matter. These waves are characterized by several fundamental parameters: density, velocity, elasticity, viscosity, structure (bulk materials, thin films), etc. [1-2]. Among dynamical techniques based on such ultrasonic waves, acoustic microscopy is the most promising one in both fundamental research and industrial applications. Such a technique [3-6] is applicable to the investigation of thin and bulk materials, the determination of materials anisotropy, homogeneity, as well as the analysis of layers/substrate structures [7-9]. These structures are characterized by two distinct effects: loading and stiffening. The loading effect appears when the propagating Rayleigh velocity in the layer, \( V_{RL} \), is slower than its counterpart that propagates in the substrate, \( V_{RS} \), subscripts L and S stand for layers and substrates, respectively. The stiffening effect is obtained when \( V_{RL} > V_{RS} \).

However, it is usually very difficult to dissociate elastic properties (density \( \rho \), and velocity \( V \)) of thin films from those of substrates onto which they are deposited. In this context, we investigate loading effects of several layers (Al, Ti, Fe, ZnO, Inconel, Crown glass, Pyrex, Heavy flint, etc.) deposited on Si and/or Mg substrates. To do so,

* Corresponding author. Tel.: + 213 38 87 27 74; fax: + 213 38 87 27 74.
E-mail address: a_doghmane@yahoo.fr

doi:10.1016/j.phpro.2009.11.041
velocity dispersion curves were first calculated, and then the optimal thickness at which thin films would behave as bulk materials were determined. Finally, analytical expressions were deduced to put into evidence the onset of bulk elastic properties.

2. Materials and methodology.

Silicon and magnesium were chosen as bulk substrates due to their multiple applications in different modern technological fields (electronic devices, communications, cellular telephony, etc.). Acoustically, Si and Mg belong to the same family, of slow materials, as far as their Rayleigh velocities, $V_R$, are concerned because $(V_R)_{Si} = 4718$ m/s and $(V_R)_{Mg} = 2930$ m/s. However, they are very different in nature; the former is the most famous semiconductor whereas the second has a good metallic behavior. The investigated thin layers (table 1) were chosen, so that loading effect condition $(V_{RL}/V_{RS} < 1)$ was verified with both substrates. Thus, we considered the following layers: Al, Ti, Fe, ZnO, Inconel, Crown glass, Pyrex, Heavy flint, etc, which are characterized by velocity ratios $0.57 < V_{RL}/V_{RS} < 0.97$ and density ratios $0.97 < \rho_L/\rho_S < 4.82$.

Simulations were carried out in the case of normal operating conditions of a conventional scanning acoustic microscope operated in the reflection mode: an operating frequency, $f = 156$ MHz, an opening angle of the acoustic lens, $\theta_{lens} = 50^\circ$ and water as the most widely used coupling liquid whose longitudinal velocity $V_{lq} = 1500$ m/s and density $\rho_{lq} = 1000$ kg/m$^3$. The methodology consists of several steps that have been described in detail elsewhere [10, 11] and will not be reiterated here; these steps can be summarized as follows: (i) calculation of acoustic materials signatures from angular spectrum model [12] (ii) determination of Rayleigh velocity via fast Fourier transform treatment of such signatures [13] (iii) application of previous to each layer thickness on both Si and Mg substrates, (iv) plotting Rayleigh velocity dependence on layer thickness for both layers/substrate structures for many layer thicknesses ranging from zero to twice the wavelength of the transverse waves propagating in the layer $(2\lambda_{TL})$ and (v) application of the above steps to the determination of the transition thickness for every plotted dispersion curve.

Table 1 Acoustic characteristics of some typical structures: thin films/substrates

<table>
<thead>
<tr>
<th>Layers/Substrates</th>
<th>Al/Si</th>
<th>Ni/Si</th>
<th>Crown/Si</th>
<th>Al/Mg</th>
<th>V/Mg</th>
<th>Inconel/Mg</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_{RL}/V_{RS}$</td>
<td>0.60</td>
<td>0.57</td>
<td>0.66</td>
<td>0.97</td>
<td>0.88</td>
<td>0.95</td>
</tr>
<tr>
<td>$\rho_L/\rho_S$</td>
<td>1.17</td>
<td>3.87</td>
<td>0.97</td>
<td>1.55</td>
<td>4.18</td>
<td>4.82</td>
</tr>
<tr>
<td>$(h/\lambda_{TL})_{tr}$</td>
<td>1.25</td>
<td>1.19</td>
<td>1.27</td>
<td>0.78</td>
<td>0.54</td>
<td>0.50</td>
</tr>
<tr>
<td>$\chi$</td>
<td>0.51</td>
<td>0.14</td>
<td>0.68</td>
<td>0.62</td>
<td>0.25</td>
<td>0.19</td>
</tr>
</tbody>
</table>

3. Velocity dispersion results

The calculated results for Al, Ni and crown glass when deposited on Si substrates are plotted in Fig. 1 in terms of Rayleigh velocity, versus normalized thickness $h/\lambda_{TL}$, for a given frequency, $f = 156$ MHz. It is clear that, unlike in bulk materials, VR in thin films is dispersive, i.e., it is a function of thickness. Moreover, all the curves possess a similar behavior consisting of an initial decrease followed by a saturation region. They all start at the same Rayleigh velocity, corresponding to that of the substrate, $(V_R)_{Si} = 4718$ m/s. Then, the decreasing region is linear with different slopes according to type of layers considered. Finally each curve saturates at a different velocity value representing the Rayleigh velocity of the considered layer when it becomes thick enough to behave as a bulk material. The latter situation occurs, graphically, at the intersection between decreasing and saturated regions (indicated by arrows in Fig. 1); it is termed as the optimal transition thickness, $(h/\lambda_{TL})_{tr}$ that is typical of each layer/Si structure (Table 1).

To enrich this investigation and to put into evidence the results reproducibility, we also considered several other layers on magnesium substrates. Typical obtained results for aluminum, inconel and vanadium are plotted in Fig. 2.
Similar behavior as that illustrated in Fig. 1 is obtained for all layers, with changing values of \( (h/\lambda_{TL})_{tr} \) from one layer to the other (see Table 1). Hence, it is clear that, with each substrate \( (h/\lambda_{TL})_{tr} \) changes with changing layers types. Thus, the good reproducibility of the results is put into evidence. Moreover, the transition thickness is not constant even for the same layer when it is deposited on a different substrate; in fact, it was found for Al layers that \( (h/\lambda_{TL})_{tr} = 1.25 \) when deposited on Si, and \( (h/\lambda_{TL})_{tr} = 0.78 \) with Mg substrates. Therefore, it can be concluded that the transition thickness depends on the properties of the substrates as well as thin layers.

**Fig. 1.** Rayleigh velocity dispersion curves as a function of normalized thickness of different layers: crown glass (●), Al (▲) and Ni (▼) on Si substrates.

**Fig. 2.** Rayleigh velocity dispersion curves as a function of normalized thickness of different layers: Al (●), Inconel (▲) and V (▼) on Mg substrates.
4. Analysis and quantification of results

A close analysis of the data in Table 1 shows that the transition thickness depends on both the characteristics of thin films and substrates. To quantify the effects of elastic parameters (velocities and densities) on the onset of thickness transition and in order to make valuable comparison between various structures and combinations, we introduce a parameter, $\chi$, defined as:

$$\chi = (V_{RL}/V_{RL})(\rho_{C}/\rho_{S})$$  \hspace{1cm} (1)

Thus, $\chi$ is a combined parameter that characterizes each layer/substrate structure. The calculated values of such a parameter, regrouped in Table 1, show that as higher $\chi$ the optimal thickness gets larger for both structures.

In order to enrich this important observation, to better understand the relation $(h/\lambda_{TL})_{tr}=f(\chi)$, to generalize this investigation and for a more precise quantification, we considered several other layers (ZnO, Ti, Cu, Fe, V, SiO$_2$, Cr, Zn, W, Duraluminium, pyrex, etc.) deposited on different substrates. It is worth noting that, to overcome the difficulties of using numerous real materials that verify loading effects with Mg substrates, and to increase the results precision, we simulated some fictitious layers, Mx$_1$ and Mx$_2$ that are characterized by the following acoustic parameters: Mx$_1$ $(V_{L}=6400 \text{ m/s}, V_{T}=2950 \text{ m/s}, V_{R}=2765 \text{ m/s} \text{ and } \rho = 4460 \text{ kg/m}^3)$ and Mx$_2$ $(V_{L}=5260 \text{ m/s}, V_{T}=2960 \text{ m/s}, V_{R}=2731 \text{ m/s} \text{ and } \rho = 3068 \text{ kg/m}^3)$, where. Dispersion curves were deduced for all these combinations which gave similar behaviors as above, namely, an initial decrease of Rayleigh velocity followed by a saturation region. The transitions occur at different $(h/\lambda_{TL})_{tr}$.

The obtained results are better illustrated in Fig. 3, in terms of the optimal transition thickness as a function of $\chi$ for Si substrates (Fig. 3a) as well as Mg substrates (Fig. 3b). It can be seen, that both cases show clearly a linear dependence; an increase of $\chi$ leads to an increase of $(h/\lambda_{TL})_{tr}$. This means that the dominance of the layers elastic characteristics whose threshold is defined by $(h/\lambda_{TL})_{tr}$ is strongly dependent on the variations in velocity and/or density of either layers or substrates. By curve fitting, it was possible to deduce this linear dependences for silicon substrates $(h/\lambda_{TL})_{Si}$ and magnesium substrates $(h/\lambda_{TL})_{Mg}$ as follows:

$$(h/\lambda_{TL})_{Si} = 1.16 + 0.16 \chi$$  \hspace{1cm} (2)

$$(h/\lambda_{TL})_{Mg} = 0.37 + 0.65 \chi$$  \hspace{1cm} (3)

These semi-empirical relations are very important in the prediction of the critical thickness beyond which any layer would behave as a bulk material. Moreover, such expressions that can be written as, $(h/\lambda_{TL})_{\text{substrate}} = \alpha + \beta \chi$ could be generalized to other types of substrates.

![Fig. 3. Variation of $(h/\lambda_{TL})_{tr}$ as a function of $\chi$ for (a) layers/Si substrates and (b) layers/Mg substrates; line of best fit (---).](image-url)
5. Conclusions

Several layers (Al, Ti, ZnO, Cu, Fe, W, Quartz, Constantan, Inconel, Crown glass, Pyrex, Heavy flint, etc.) deposited on Si and/or Mg substrates were investigated. From the calculated dispersion curves of Rayleigh velocity, the transition thickness \((h/\lambda_{TL})_{tr}\) separating layer characteristics from those of the substrates was deduced. To analyze and quantify the results we introduced a parameter \(\chi\) that takes into account velocities and densities of layers and substrates to finally deduce relations of the form \([(h/\lambda_{TL})_{tr}]_{\text{substrate}} = \alpha + \beta \chi\) that could be applied to any combination. These expressions would give a better understanding of the propagation of surface acoustic waves in thin films and bulk materials.

References