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A study of the morphology of thin films by surface acoustic wave pulses♣

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Changes arising in the dispersion and attenuation of short surface acoustic wave (SAW) pulses, caused by material elastic and density imperfections and discontinuities, are discussed from the viewpoint of using them for inspecting the morphology and homogeneity of thin amorphous films. For this purpose, one can relate variations in the frequency dependence of the SAW phase velocity and attenuation coefficient with parameters describing the surface roughness profile. The approach is demonstrated via an example of the determination of the morphology of a thin film of a-Si:H deposited by laser-induced chemical vapour deposition (LICVD) on a c-Si substrate.

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1. Introduction

The microstructure and homogeneity (morphology) of a thin solid film determines its physical properties, and because surface acoustic waves (SAW) are quite effective in probing it, attempts to use SAW attenuation and dispersion due to scattering on surface roughness and discontinuities have been undertaken, both theoretically and experimentally [1-4]. To relate the SAW dispersion and attenuation to the film morphology, one needs both realistic models for the mechanisms of the wave interaction with the film material and suitable effective parameters describing the main peculiarities of the film morphology. This paper proposes how one can relate the routinely observable parameters of the propagation of short SAW pulses to specific features of the microstructure of a thin amorphous film.

2. Theoretical model

For amorphous materials at room temperature, the main mechanism of attenuation of SAW in the frequency range below about 1 GHz is scattering due to surface discontinuities. Three types of these have been treated theoretically so far: (i) surface point mass defects [1,5], (ii) surface fluctuations in the mass-density and the Lame coefficients of the film [2], and (iii) surface roughness [3,4,6]. In what follows, we summarize briefly the main results concerned.

(i) *Mass-defects*:

A localized (point) mass defect Δm, situated either at the surface or close to it, scatters SAW in a manner described by the attenuation coefficient

$$\alpha = 0.08\, c(\Delta m)^2\omega^5/\rho^2 V_R^5 \qquad (1)$$

where ρ is the film density, c the concentration of defects per unit area, ω the radian frequency and $V_R = \omega/k$ the velocity of the Rayleigh wave. The assumption made in determining the numerical factor in (1) is a Poisson's ratio of 0.29. If more than one type of mass defect is present at the surface, a "mass-roughness" parameter $R = \Sigma_i\, c_i\, (\Delta m_i)^2$ can be introduced into (1), summed over obstacles of all sizes. Obviously, by presenting the surface point-mass defects in the form [5]

$$\rho(\boldsymbol{r}) = \langle\rho\rangle + \Delta m\, D(\boldsymbol{r}) \qquad (2)$$

where $\langle\rho\rangle$ is the averaged mass-density, $\boldsymbol{r}$ a two-dimensional position-vector in the plane of SAW propagation, and $D(\boldsymbol{r})$ the fluctuation distribution function, one can treat the point mass defects as surface density fluctuations, or vice versa. The main advantage of this model is that it makes use of phenomenological

♣ Paper presented at the International School on Condensed Matter Physics, Varna, Bulgaria, September 2008 parameters such as the defect masses and concentrations, rather than of correlation functions. At the same time, at least as far as the frequency dependences of the SAW propagation parameters are concerned, both approaches give the same results.

(ii) *Effect of surface roughness*

In an isotropic elastic medium bounded by a flat surface, the velocity of a Rayleigh wave, $V_R^0(k)$, does not depend on frequency (the no-dispersion case). If the surface is rough, a downward shift of the SAW velocity arises, given by

$$V_R(k)/V_R^0(k) = \Delta\omega(k)/\omega_o(k) \equiv \omega(k)/\omega_o(k) - 1 \quad (3)$$

Here, $\Delta\omega(k)$ is the surface-roughness-induced complex dispersion relation (the shift of the SAW frequency away from its value for a flat surface, $\omega_o(k)$) and $\boldsymbol{k}$ is a two-dimensional wave-vector. Based on detailed theoretical grounds [3], the real part of (3) is

$$\mathrm{Re}\{\Delta\omega(k)/\omega_o(k)\} = (\delta/a)^2\, \Omega_1(ak) \quad (4a)$$

while its imaginary part determining the attenuation coefficient α of the Rayleigh wave, is

$$\alpha \equiv \mathrm{Im}\{\Delta\omega(k)/\omega_o(k)\} = 2(\delta/a)^2\, k\, \Omega_2(ak) \quad (4b)$$

Thus, both the SAW attenuation and the dispersion can be expressed in terms of two "universal" functions, $\Omega_1(ak)$ and $\Omega_2(ak)$, and the ratio (δ/a), describing entirely the rough-surface profile. (Here, δ is the root-mean-square departure of the surface from flatness, and a is the transverse correlation length that describes the average distance between successive peaks and valleys in the rough-surface profile.) The general explicit form of both functions is quite complicated and cumbersome to treat otherwise than numerically, when the argument varies in a large interval. However, for small values of ak (or $2\pi a/\lambda$, λ is the SAW wavelength), the case met for frequencies up to a few GHz, these functions can be approximated by simple analytical expressions. For example, $\Omega_2(ak) \sim (ak)^4 \sim \omega^5/V_R^5$ for $ak \ll 1$, leading to the same fifth-power dependence of α on frequency as that given by (1). This fact makes it possible to unite into a factor the diverse mechanisms of SAW attenuation. The exact behavior of the functions $\Omega_1(ak)$ and $\Omega_2(ak)$, for ak-values of interest for this study, is shown Figs. 1 and 2, respectively.

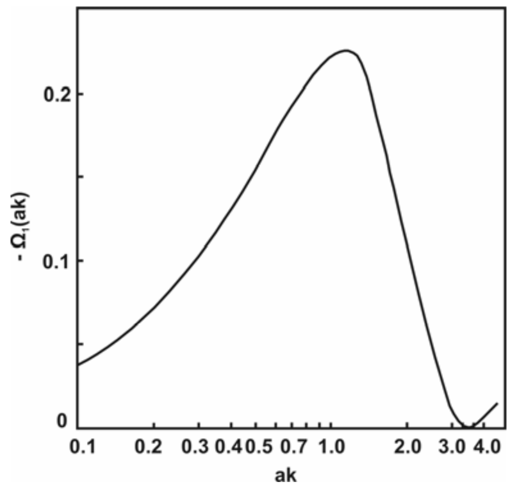

Fig. 1. Behaviour of the function $\Omega_1(ak)$

On the other hand, the presence of a thin layer of different material on the surface leads to SAW dispersion, even if both the substrate and the layer are ideally isotropic and homogeneous [7,8]. In many cases, however, especially where amorphous and coarse-grain structured films are concerned, this approach has failed to give a good fit to the experimental dispersion curves, at least for a substantial part of the frequency range studied. A very probable reason for such a disagreement might be an additional change of the SAW phase velocity induced by the film surface roughness and heterogeneous morphology, as well as by imperfections and discontinuities at the film-substrate interface.

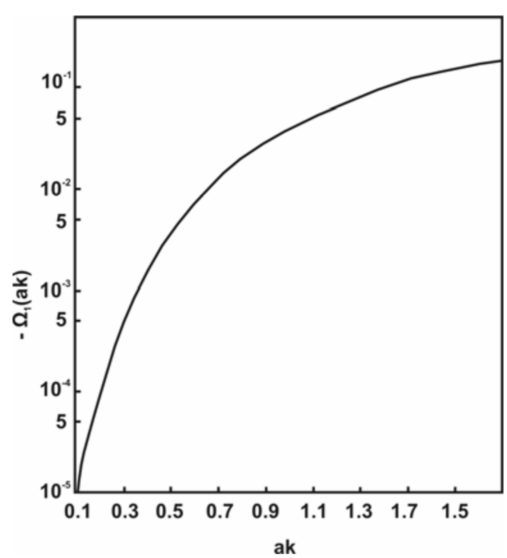

Fig. 2. Behaviour of the function $\Omega_2(ak)$

3. Experimental example

For details of the experimental method used in obtaining the discussed data, see [9]. The SAW pulses were excited by a XeCl excimer laser (20 ns pulse duration, 308 nm wavelength) focused on the sample's surface to a line of 10-20 μm width and 20 mm length. The linear focus scans the surface with a precision of about 2 μm. After propagatingover a distance of between 5 and 30 mm, the excited SAW pulses were detected either optically by a Michelson's interferometer or by a piezoelectric PVDF foil transducer (with a measurement bandwidth of about 100-200 MHz and a maximum sensitivity of about 0.2 Å). For determining the SAW dispersion and attenuation, we averaged several thousand pulses in the time domain, and converted the signal into the frequency domain by Fourier transformation.

The investigated a-Si:H films were deposited on the (100)-plane of Si wafers by laser-induced chemical vapour deposition (LICVD), using a cw CO_2 laser beam parallel to the substrate surface. The films were between 0.5 and 1.6 μm thick and contained between 5% and 17% hydrogen (the SAW was excited in the [001]-direction of the (100) plane, parallel to the axis of the deposition laser beam) [10].

We used these experimental data to illustrate how the proposed approach for studying thin amorphous films works.

Fig. 3 presents the frequency dependencies of the SAW phase velocity (left-hand side scaled) and attenuation coefficient (right-hand side scaled) for a 1.15 μm thick *a*-Si:H film with 7% hydrogen content, deposited at a substrate temperature of 350°C. The solid lines show the experimentally measured dependencies, while the dotted ones are the best fits to the attenuation curve and to the high-frequency part of the SAW phase velocity dispersion. The dashed line in Fig. 3 presets the best fit to the low-frequency part of the dispersion curve, obtained using a second-order perturbation method [9]. We were not able to find any set of reasonable values for the fitting parameters (including also the film density) in order to obtain a satisfactory fit of the dispersion curve in the whole frequency range studied. The stepwise change in curvature, experimentally observed at about 35 MHz in the $V_R(\omega)$ curve, could not be explained by any known model of SAW dispersion in a thin homogeneous film on an isotropic substrate. (These models are valid only for small values of kh, where h is the film thickness, which was the reason to fit in this way the low frequency part of the curve.) At the same time, we succeeded in fitting very well the high-frequency part of this curve using (4a) and the function $\Omega_1(ka)$ in Fig. 1 (shown by the dotted line in Fig. 3). The parameters obtained by such a fitting procedure are $\delta/a = [0.122 \pm 0.002(5)]$, $a = 7.75\ h \approx 9$ μm, and $\delta = 0.95\ h \approx 1$ μm. The inaccuracy in determining δ and a separately comes from that in determining the film thickness h.

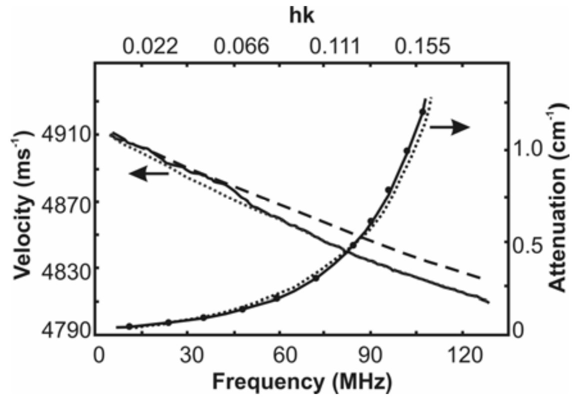

Fig. 3. SAW phase velocity V_R (left-hand side scaled) and attenuation coefficient α (right-hand side scaled) as functions of the frequency ω. Solid lines – experiment, dotted lines – fits to experimental data in the whole frequency range for α and to the high frequency region for V_R, dashed line – fit to the low-frequency region of V_R using a second order perturbation method.

Similar results are obtainable by fitting the curve α(ω) in Fig. 3 using (4b) and the function $\Omega_2(ka)$ in Fig. 2 (the.dotted line in Fig. 3). In this case, $\delta/a = [0.138 \pm 0.005(7)]$, $a = 7.84\ h \approx 9.1$ μm, and $\delta = 1.08\ h \approx 1.1$ μm, i.e. essentially the same values of δ and a, although within a more than twice poorer accuracy.

3. Conclusions

The change of short SAW pulses caused by diverse material discontinuities, which varies as the fifth (or close to the fifth) power of frequency, are adequately described in terms of various *surface "roughness"* contributions. Such an approach to the averaged *overall* SAW dispersion and attenuation is suitable for inspecting the morphology of thin films and solid surfaces. Both the SAW dispersion and the attenuation caused by surface roughness are equally informative in terms of the dimensionless ratio δ/a, the two parts of which can accurately be determined by fitting experimental curves, provided the film thickness is measured independently.

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