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Three-Phase Model for the Volmer-Weber Crystal Growth

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Thin film deposition is a widely used technique for the fabrication of MEMS (Micro-Electro-Mechanical Systems) devices. This technique is required to establish free-standing structures which can induce or sense a mechanical movement. During the deposition of new layers of thin films an intrinsic stress is generated. In subsequent process steps, a stressed layer, usually an important component part of the desired MEMS device, is left free-standing. As a consequence the process induced stress can relax and deform the layer in an undesirable way. For the investigation of stress effects during deposition we are focusing on the deposition of SiGe on the sacrificial layer. In our model we combine three stress generation mechanisms where each is related to one of three charachteristic phases of thin film growth and corresponding microstructure evolution. In the initial phase we assume the so-called Volmer-Weber growth which includes a build-up of a strong compressive stress components due to the Laplace pressure of isolated material islands [2]. It is followed by a tensile stress mechanism which operates during the island coalescence phase and thereafter [2]. The third phase introduces again compressive component but this time due to adatom insertion into the top of the grain boundaries (Figure 1). The basic feature of our approach is an introduction of the strain-gradient function $\omega(z,r)$ which depends on the grain size distribution function $L(z)$ and material deposition rate r. $L(z)$ can be obtained by using several different algorithms which simulate morphology evolution of the thin film microstructure according to the Van der Drift mechanism [3]. The first expression in (1) ($\varepsilon(z,r)$) represents the microstrain evolution in the direction of the film growth (Figure 1). It consists of the strain contribution from the first phase $\varepsilon_{t,1}(z_i,r)$, where z_i is the film thickness after a coalescence, and an integral term relating to microstrain development in the second and the third phase (1),

$$\varepsilon(z,r) = \varepsilon_{t,1}(z_i,r) + \int_{z_i}^{z} \omega(w,r)\,dw, \quad \omega(z,r) = \omega_{t,2}(z,r) + \omega_{c,3}(z,r). \tag{1}$$

The strain-gradient function $\omega(z,r)$ consists of a tensile ($\omega_{t,2}(z,r)$) and a compressive ($\omega_{c,3}(z,r)$) component. The third phase compressive contribution $\omega_{c,3}(z,r)$ (2) depends on the jumping frequency Γ_c of adatoms into a grain boundary and adatom concentrations C_a, C_0, at the top of the grain boundary and elsewhere on the grain surface, respectively [2]. ε^* is the local strain at the top of the grain and $\beta = \Omega M/kT$ [2].

$$\omega_{c,3}(z,r) = -\frac{2\,\Omega\,\Gamma_c}{L(z)\,r}\Big(C_a - C_0\,e^{-\beta\varepsilon^*}\Big) \tag{2}$$

We have applied our model for Poly-SiGe PECVD thin film deposition [4]. For an experimental thin film deflection a microstrain curve has been extracted in our previous work [1]. The comparison between this experimental microstrain and the microstrain obtained by the presented three-phase model is given in Figure 2. Since the model explicitly includes both process and material parameters, it can readily be used to improve the mechanical behavior of thin films. For example, a compensation effect [4] of top layers can be enhanced by increasing the compressive component $\omega_{c,3}(z,r)$ induced in the third phase by means of a reduction of the deposition rate r (2).

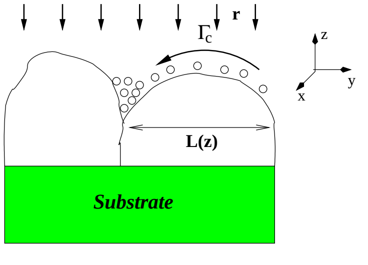

Figure 1: Third phase. Adatoms are inserted between the grain boundaries.

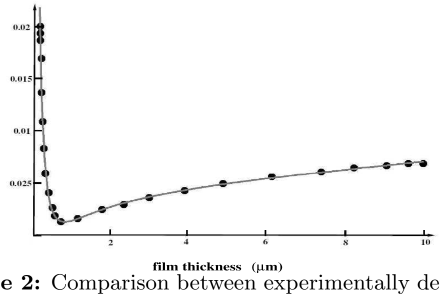

Figure 2: Comparison between experimentally determined microsrains (dots) with simulation (full-line).

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