Intrinsic Stress Build-Up During Volmer-Weber Crystal Growth

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Abstract

We present a model for build-up of intrinsic stress during the deposition of thin metal films. The model assumes a three-phase stress generation mechanism which corresponds to three characteristic phases of microstructure evolution. The simulation results based on the model are successfully compared with experimental results for Poly-SiGe PECVD films. The impact of critical parameter variation on mechanical properties of thin film is discussed.

1 Introduction

Residual mechanical stress introduced during deposition of thin films and coatings has a significant impact on the reliability of electronic devices and structural components. The mechanical stress in thin metal films consists of a thermal component and an intrinsic component due to the evolution of the metal microstructure during film growth. The goal of this work is the integration of the respective models for the specific phases of microstructural evolution into a comprehensive model which describes the intrinsic stress behavior during the entire deposition process. This model can be used to assess and optimize the mechanical stability of multilayer structures.

2 Theoretical Considerations

The model introduced here is based on the work presented in [1, 5, 6]. For the sake of generality we define our model in the sense of strain which is developed during the deposition of a metal film due to microstructural evolution. We combine three microstrain generation mechanisms, each arising in the characteristic phase of thin film growth (Fig. 1).
In the initial phase we assume the so-called Volmer-Weber growth which includes a build-up of a strong compressive stress component due to the Laplace pressure of isolated material islands [1]. It is followed by a tensile stress mechanism which operates during the island coalescence phase and thereafter [1]. The third phase introduces again a compressive component, but this time due to adatom insertion into the top of the grain boundaries (Fig. 2). 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 the morphology evolution of the thin film microstructure according to

the Van der Drift mechanism [7]. An example concerning the Van der Drift growth for a representative group of 9 grains is given in Fig. 3 and Fig. 4. The evolution of the microstrain $\varepsilon^I(z,r)$ in the direction of the film growth is given by (1). The microstrain consists of the 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 (2),

$$\varepsilon^I(z,r) = \varepsilon_{t,1}(z_i,r) + \int_{z_i}^{z} \omega(w,r)\,dw, \tag{1}$$

$$\omega(z,r) = \omega_{t,2}(z,r) + \omega_{c,3}(z,r). \tag{2}$$

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 $\omega_{c,3}(z,r)$ (3) depends on the jumping frequency Γ_c of adatoms into a grain boundary (Fig. 2) and adatom concentrations C_a, C_0, at the top of the grain boundary and elsewhere on the grain surface, respectively [1]. ε^* is the local strain at the top of the grain and $\beta = \Omega M/kT$ [1].

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

The straightforward way to apply a microstrain model on larger multilayer structures is given by using linear elastic theory. In this case the microstrain acts as residual stress,

$$\sigma(x,y,z) = \mathbf{D}(\varepsilon(x,y,z) - \varepsilon^I(z,r)\mathbf{I}). \tag{4}$$

The overall mechanical problem is defined by the equilibrium condition $\nabla\sigma = 0$. The obtained system of partial differential equations is solved by means of the finite element method.

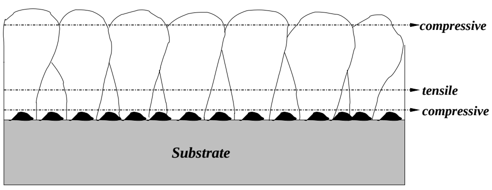

Figure 1: V-shape grain growth.

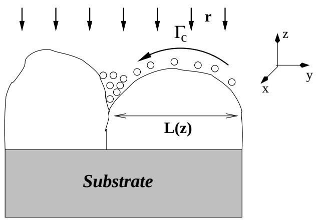

Figure 2: Third phase. Adatoms are inserted between the grain boundaries.

3 Simulation Results and Discussion

Since our model is defined for general Volmer-Weber crystal growth, it can be applied for a multitude of different metals and deposition processes. For example, a well established fact is that AlN, copper, and SiGe thin films deposited on a Si/SiO_2 layer exhibit Volmer-Weber growth with three distinctive stress generation phases ([1, 3, 6]).

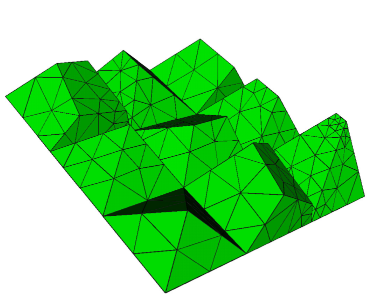

Figure 3: Grains after coalescence.

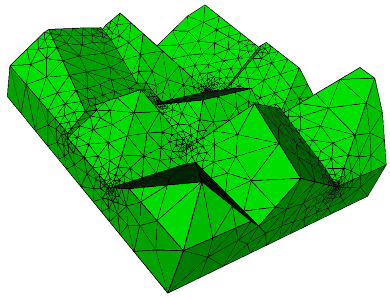

Figure 4: Grains after Van der Drift growth.

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 [2]. The comparison between this experimental microstrain and the microstrain obtained by the presented three-phase model is given in Fig. 5. Three phases of the microstructure are clearly recognizable in the microstrain curve. The resulting profile lays completely in the area of compressive strain, because the compressive contribution dominates over tensile one. In the first part of the microstrain curve (Fig. 5), a high compressive component from the first phase can be seen. The curve further sinks (but it remains positive) indicating an impact of the tensile component which bears a negative sign. Continued growth of V-shaped grains introduces a final compressive component

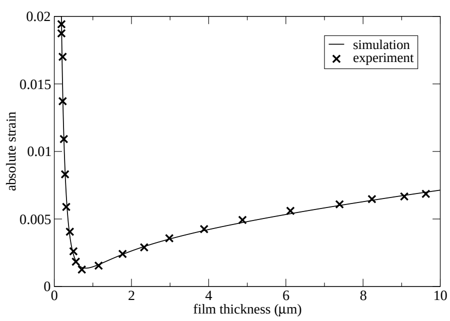

Figure 5: Comparison between experimentally determined microstrain with simulation.

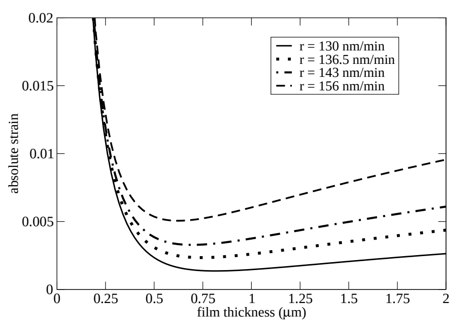

Figure 6: The effect of deposition rate variation.

of the third phase. Numerous experimental observations have shown that the variation of process conditions of SiGe PECVD after reaching the third phase [3] does not disrupt the growth of individual grains. Changing the deposition rate or germanium concentration can increase or reduce the number of adatoms arriving at the top of the grain boundary, the mobility of the adatoms can be influenced by changing process temperature and germanium concentration, but grains continue their growth [3]. However, measurements clearly show that the resulting strain in the film changes. The effect of the deposition rate variation on microstrain is given in Fig. 6. From this picture we can conclude that increasing the deposition rate enhances the compressive component from the third phase of the growth process. Increasing of the deposition rate to 5 %, 10 %, and 20 %, causes an increase of the third phase compressive component to 65 %, 131 %, and 263 %, for 2 μm film thickness, respectively. This effect can be practically used for design of the so-called compensation layers at the final stage of thin film deposition for MEMS applications [3].

4 Conclusion

In this work we have presented a three phase model for evolution of microstrains in deposited thin metal films. Since our model considers a general dynamics of formation and evolution of grains, it can be applied to a wide spectrum of technological processes and materials. The model is designed as a combination of previously studied and published models for separate phases of the microstructure evolution.
Intrinsic residual microstrains are used to raise the mechanical problem to a larger scale and to model the behavior of complex multilayer films. We have calibrated our model using measurements of SiGe PECVD thin film (cantilever) deflection. The theoretically obtained microstrain curve reproduces very well experimental results. Finally, we have investigated the impact of a process parameter variation on the microstrains. Since the model explicitly includes both process and material parameters, it can readily be used to improve the mechanical behavior of thin films.

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