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Residual stresses in thin film systems: Effects of lattice mismatch, thermal mismatch and interface dislocations

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ABSTRACT

This paper explores the mechanisms of the residual stress generation in thin film systems with large lattice mismatch strain, aiming to underpin the key mechanism for the observed variation of residual stress with the film thickness. Thermal mismatch, lattice mismatch and interface misfit dislocations caused by the disparity of the material layers were investigated in detail. The study revealed that the thickness-dependence of the residual stresses found in experiments cannot be elucidated by thermal mismatch, lattice mismatch, or their coupled effect. Instead, the interface misfit dislocations play the key role, leading to the variation of residual stresses in the films of thickness ranging from 100 nm to 500 nm. The agreement between the theoretical analysis and experimental results indicates that the effect of misfit dislocation is far-reaching and that the elastic analysis of dislocation, resolved by the finite element method, is sensible in predicting the residual stress distribution. It was quantitatively confirmed that dislocation density has a significant effect on the overall film stresses, but dislocation distribution has a negligible influence. Since the lattice mismatch strain varies with temperature, it was finally confirmed that the critical dislocation density that leads to the measured residual stress variation with film thickness should be determined from the lattice mismatch strain at the deposition temperature.

1. Introduction

Driven by the increasing demand for faster microprocessors and packing more transistors on a single chip, silicon-on-insulator (SOI) systems have been found a technology to extend the Moore's law in the coming decades (Celler and Cristoloveanu, 2003). However, due to the difference in thermal and mechanical properties of silicon and insulating substrate, residual stresses in vapor deposited layers, by either physical or chemical methods, are inevitable. Such stresses could induce crystallographic defects, leading to higher resistance to the transportation of carriers or phonons, or macroscopic defects, such as buckling, cracking, and delamination, leading to the failure. Hence, understanding the origin of the residual stress variations in such systems is essential.

There are two primary causes of residual stresses in an SOI thin film system. The first is thermal mismatch. When a system is cooled down from a deposition temperature to room temperature, the mismatch of the coefficients of thermal expansion (CTE) of the thin film and the substrate leads to residual stresses in the system. The second cause is the dissimilar lattice structures of the materials, which leads to residual stresses and lattice defects.

Some theoretical and experimental methods have been proposed in the literature to calculate the residual stresses induced by lattice and thermal mismatches and to investigate the stress release by dislocations. Experimentally, these include the methods with the aid of beam curvature (Dumin, 1965), Raman (Englert et al., 1980; Wang et al., 2005) spectroscopy and X-ray diffraction (Liu et al., 2010; Vreeland and Paine, 1986). However, the total residual stresses measured by the experimental methods cannot distinguish the contributions by the mismatches of CTE and lattice structures as well as by the relaxation due to lattice defects.

After the first analytical model developed by Stoney in the early 1900s (Stoney, 1909), a great number of theoretical studies have been conducted, trying to improve the Stoney's equation for calculating the residual stresses in a thin film system. For instance, Timoshenko (1925), Rich (1934) and Klein (2000) relaxed the assumption of negligible film thickness. Freund (2000) considered the effect of finite strain and rotation. Freund and Suresh (2003) removed the assumption of a uniform stress distribution in a thin film. Hu and Huang (2004) investigated the elastic and elastoplastic multilayer thin film systems, and Huang and Rosakis (2005) further extended the Stoney's formula to be applicable to a non-uniform temperature distribution in a thin film substrate system.

Many analytical solutions have also been proposed for calculating the stresses due to misfit dislocations. Vandermerwe (1950) solved the stresses, atomic displacement and energies due

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to a single misfit dislocation on the interface of two crystals of different lattice spacing. Further developments have afterwards been made to calculate distributions of elastic strains and internal stresses in thin epitaxial films deposited on dissimilar substrates (Ball, 1970; Ball and Van der Merve, 1970; Bonnet, 1996; Jesser and Matthews, 1967, 1968a,b; Matthews, 1968; Matthews and Crawford, 1970; Nakahara, 1989; van der Merwe, 1964; Yao et al., 1999). Gutkin and Romanov (Gutkin et al., 1993; Gutkin and Romanov, 1991, 1992a,b) considered the effects of dislocation interactions, free surface and far field stresses, which were neglected in previous theories and presented a continuum mechanics solution for the stress field around a straight edge dislocation in the interface of two heteroepitaxial materials, applicable directly to a film-on-substrate system. Such analytical models are often complicated in mathematical formulation.

Making use of the stress or strain field surrounding dislocations, the thickness-dependent lattice relaxation was considered (Ayers, 2007). Matthews and Blakeslee (1974) considered the force equilibrium of a threading dislocation and resulted in that the lattice relaxation was inversely proportional to the film thickness. Matthews et al. (1970) included the Peierls force (lattice friction force) in the model and resulted in the kinetic relaxation of lattice strain. Dodson and Tsao (1987) later included the effect of dislocation multiplication and resulted in a more empirical model. All these models, however, were on small lattice mismatch strain (less than 1%), which makes the assumption of small deformation valid and the analytical treatments possible. For the epitaxial thin film system of relatively large mismatch strains, including the silicon-on-sapphire (SOS) system to be considered in the present work, the thickness-dependent lattice relaxation has not been explored. This could be due to the difficulty when the strain is large and when the change of growth mode from layer-by-layer growth to island growth comes into play. It was also noted that for the large mismatch strain in the SOS system, the critical film thickness (at which the first misfit dislocation nucleates) is much less than 10 nanometres according to the theory (cf. e.g., "Heteroepitaxy of Semiconductors" by Ayers). In this case, the film actually grows through domain epitaxy (cf. e.g., Narayan and Larson, 2003; Bayati et al., 2012) and island coalescence (cf. e.g., Hamarthibault and Trilhe, 1981). The misfit dislocations form spontaneously inside islands or during island coalescence (cf. e.g., Legoues et al., 1994; Qian et al., 1997). The classical models based on kinetics of dislocations may not be necessary. Instead, one may directly model the misfit dislocations at the interface and study their influence through elastic analysis of dislocations.

Owing to the fast increase of computational capacity, the finite element (FE) method has become an efficient tool to study the residual stresses attributed to the combined effects of CTE and lattice mismatches as well as the relaxation due to lattice defects. A number of studies have been carried out using the FE method to understand the residual stresses in film-on-substrate systems due to CTE mismatch (Gu and Phelan, 1998; Han et al., 2009; Wright et al., 1994). The focus of these studies was on the effect of deposition temperature, but the simulations were based on two dimensional (2D) models considering only isotropic temperature-independent material properties. A more comprehensive investigation was conducted by Pramanik and Zhang (2011) who carried out a three dimensional (3D) finite element analysis of the thin film residual stresses. In their study, however, the effects of lattice mismatch and dislocations were not included. In our previous study (Liu et al., 2012), it was experimentally found that the residual stress in the silicon film for a silicon-on-sapphire system depends on the film thickness even when the film thickness was of hundreds of nanometres. This result cannot be explained by merely the CTE mismatch. Therefore, a more thorough study is necessary to clarify the origin of residual stress in the thin film.

The aim of this paper is to make a major step forward to reveal the origin of residual stress variation in film-substrate systems when thermal and lattice mismatches and multiple lattice defects come into play all together. To explore the effect of the individuals, and hence to uncover the variation mechanisms of the residual stresses, the contributions of CTE and lattice mismatches and misfit dislocations will be investigated step-by-step.

2. FE modeling

Among the various insulating materials practiced by the semiconductor industry, we consider sapphire in this study. This is because sapphire has recently won a broad acceptance in commercial applications due to its low power consumption and efficient insulating properties. In the silicon-on-sapphire (SOS) technology, a thin hetero-epitaxial silicon layer grows on sapphire at a high temperature. A mono-crystalline sapphire structure has been shown in Fig. 1. To minimize the effect of lattice mismatch between silicon and sapphire, the (1 0 0) silicon layer is normally deposited on to the $(1\bar{1}02)$ plane (R-plane) of sapphire (Nakamura et al., 2004). The silicon properties are considered to be orthotropic, whereas the sapphire is regarded as an anisotropic material whose stiffness matrix (Goto et al., 1989) can be converted to the coordinate system indicated in Fig. 1 (i.e., the *x*, *y*, *z* axes are respectively $[\bar{1}101]$, $[11\bar{2}0]$ and $[1\bar{1}02]$). The thermal and mechanical properties of silicon and sapphire are listed in Appendix A.

A schematic of the 3D FE model for investigating the residual stresses in an SOS system is shown in Fig. 2. The model shape resembles an SOS wafer to include all the possible geometrical effects (Moridi et al., 2011). A volume of interest (VOI) is defined in the centre of the model with the finest mesh as shown in Fig. 2. To avoid the boundary effect, the radial dimension of the model was 30 times the thickness of the thin film. Overall, the VOI contained 4440 elements, and the whole model consisted of 34,628 elements. A mesh sensitivity test confirmed that this mesh density was sufficient. The finite element model was solved by ANSYS V12.1 with the 10-noded SOLID 98 elements which can cope with both thermal and mechanical responses.

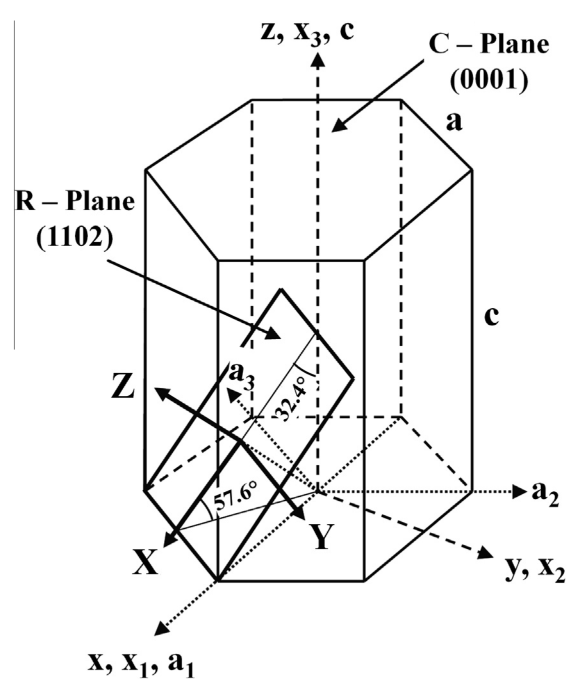

Fig. 1. Coordinate systems in the sapphire crystal and in the $(1\bar{1}02)$ plane.