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Thermo-mechanical constitutive equations for glass and its numerical formulation for warpage analysis of silicon-glass multilayered structure

Ji Hoon Kim [a], [*], Kwansoo Chung [b], [*]

[a] School of Mechanical Engineering, Pusan National University, 2 Busandaehak-ro 63beon-gil, Busan 609-735, Republic of Korea
[b] Department of Materials Science and Engineering, Research Institute of Advanced Materials, Engineering Research Institute, Seoul National University,
599 Gwanak-ro, Gwanak-gu 151-744, Republic of Korea

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ABSTRACT

Thin multilayered structures with glass substrates are widely used in electronic devices. When layers having different thermal or mechanical properties are subjected to processes with temperature variations, warpage and residual stresses may develop incurred by the mismatch of volume change, possibly leading to the failure of the device. In order to analyze the thermo-mechanical behavior of glass including the warpage in multilayered structures with glass substrates, the thermo-mechanical constitutive equations of glass are developed here by coupling the stress relaxation (for mechanical behavior) and structural relaxation models (for thermal behavior). The constitutive equations for structural relaxation are generalized for the case with temperature dependent thermal expansion coefficients, while considering both formulations based on the specific volume and the fictive temperature. Besides, the numerical formulations of the constitutive equations for finite element analysis are derived for three-dimensional and plane stress conditions. The developed constitutive model is validated with experiments for the warpage of silicon-glass multilayered structures undergoing thermal cycles.

1. Introduction

Most electronic devices are made of layers of different materials laminated by deposition or bonding. For example, flat panel displays (Burrows et al., 1997; Ellison and Cornejo, 2010; Park et al., 2012) and microsensors (Chang et al., 2009; Kim et al., 2011) are composed of glass, polymer, metal, and/or ceramic layers with thicknesses ranging from a few nanometers to millimeters. The layers composing electronic devices often have different thermal, mechanical and chemical properties. Thus, upon the change of thermal environment, bending of the layers, or warpage, may occur along with residual stresses caused by mismatch of volume change induced by thermal expansion or structural change such as curing. In most cases, warpage has detrimental effects on structural integrity, often leading to the failure of the device.

When temperature is kept much lower than the melting temperature for crystalline materials or the glass transition temperature for amorphous materials, the behavior of materials usually follows linear elasticity and linear thermal expansion in mechanical and thermal behaviors, respectively, such that the elastic analysis is suitable to examine the warpage of layered structures. Stoney (1909) has developed an analytical equation for calculating the bending stress of an infinitely thin film

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[*] Corresponding authors.
E-mail addresses: kimjh@pusan.ac.kr (J.H. Kim), kchung@snu.ac.kr (K. Chung).

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deposited on a substrate from the curvature of the substrate using the linear elasticity theory. This equation has been used and further modified in many works ensued (Flinn et al., 1987; Janssen et al., 2009). Timoshenko (1925) and Freund et al. (1999) have developed analytical relationship between the curvature and the stress for a layered structure with a finite thickness ratio of the film to the substrate. Lim et al. (2007) have calculated the warpage of adhesively bonded Si and glass wafers by thermal loading based on linear elasticity. Numerical methods are often introduced to solve more complex problems. Che et al. (2011) have developed a thermo-mechanical model to predict the warpage of Si wafers with Cu layers for electronic packaging by applying linear elasticity and the finite element method.

Electronic devices often undergo heating and cooling cycles during manufacturing processes. If amorphous materials such as glass and polymer are used as layers and the layered structure is subjected to a temperature change near the glass transition point, the elastic analysis may be no longer applicable because these materials exhibit viscoelastic mechanical and nonlinear thermal behaviors. More specifically, for amorphous materials, stress decreases gradually with time upon a deformation by an applied loading, which is known as stress relaxation (Le Bourhis, 2008; Huang et al., 2011). Also, the specific volume of amorphous materials is affected by both the thermal vibration and microstructural rearrangement. The microstructural rearrangement is a time-dependent process: the viscosity of amorphous materials drags atoms movement and rotation, hindering the rearrangement toward a thermo-dynamically stable microstructure. This time-delayed irreversible thermal response is known as structural relaxation (Angell et al., 2000). Therefore, the structural relaxation as well as the stress relaxation should be properly accounted for to analyze thermo-mechanical behaviors including the warpage of multilayered structures with amorphous materials such as glass.

Earlier works on viscoelasticity include the development of the constitutive equations for stress relaxation (of the mechanical behavior) (Lee et al., 1965; Knauss and Emri, 1981) and their numerical implementations for finite element calculation (Scherer and Rekhson, 1982; Chambers and Becker, 1986; Chambers, 1992). As for nonlinear thermal expansion, the structural relaxation model (of the thermal behavior) has been first introduced by Tool (1946) and further developed by Narayanaswamy and coworkers (Gardon and Narayanaswamy, 1970; Narayanaswamy, 1971, 1978, 1988). In recent years, advanced constitutive models and material parameter characterization techniques were introduced for studying the viscoelasticity. Abu Al-Rub and Darabi (2012) and Darabi et al. (2012) formulated a robust constitutive model incorporating viscoplasticity, viscodamage, and micro-damage healing as well as viscoelasticity based thermodynamics. Zhu and Sun (2012) derived a viscoelastic-viscoplastic damage constitutive model based on the irreversible thermodynamics theory. Zaïri et al. (2011) developed a physically-based model for rubber-toughened glassy polymers using the hyperelastic-viscoplasticity and visco-hyperelasticity. The time-dependent mechanical behavior of polymers (Ayoub et al., 2011; Shim and Mohr, 2011) and rubber-like materials (Ayoub et al., 2014) were studied for large cyclic strains. The transient and steady-state creep behavior of polymeric materials was measured using the nanoindentation technique and the results were analyzed by the viscoelastic model (Huang et al., 2011). Grassia and coworkers (Grassia and D'Amore, 2010, 2011; Grassia et al., 2011, Grassia and Simon, 2012) proposed a constitutive model for expressing the PVT and volume relaxation of polymeric materials by extending the structural relaxation model originally developed by Kovacs et al. (1979).

A viscoelastic stress relaxation model has been applied to study warpage in multilayered structures with amorphous materials. Yang et al. (2003) have used a cure-dependent viscoelastic constitutive model to minimize the warpage of a polymer-steel layered structure. Lin and Lee (2008) have developed a viscoelastic warpage model of the epoxy laminated packaging. Komoto (2010) has calculated the warpage of the molding compound on a substrate by the viscoelasticity and the finite element method. Jansen et al. (2011) have estimated cure-induced stresses and warpage in layered structures by applying the viscoelasticity to the polymeric mold compound. In these works, the stress relaxation has been found to affect the stress strongly. All these works, however, have not considered the effect of structural relaxation on the warpage of multilayered structures.

In this work, the thermo-mechanical constitutive equations for glass are derived to account for both the stress relaxation and structural relaxation behaviors. As for the structural relaxation model, both models based on the specific volume and the fictive temperature are considered. In addition, the structural model is generalized for cases with temperature dependent thermal expansion coefficients. Besides, the numerical formulations of the developed constitutive models for finite element analysis are derived for three-dimensional and plane stress conditions. The warpage of the Si-glass multilayered structure undergoing thermal cycles is analyzed using the developed constitutive model, which is also experimentally validated.

2. Thermo-mechanical constitutive equations of glass

The total strain rate tensor may be decomposed into the thermal and mechanical strain rate tensors. The mechanical strain rate tensor may be further decomposed into the mechanical volumetric and deviatoric strain rate tensors; i.e.,

$$\dot{\varepsilon}_{ij} = \dot{\varepsilon}^{th}_{ij} + \dot{\varepsilon}^{m}_{ij} = \dot{\varepsilon}^{th}_{ij} + \dot{\varepsilon}^{mv}_{ij} + \dot{e}_{ij},\ (i,j = 1,2,3) \tag{1}$$

where $\dot{\varepsilon}_{ij}$, $\dot{\varepsilon}^{th}_{ij}$, $\dot{\varepsilon}^{m}_{ij}$, $\dot{\varepsilon}^{mv}_{ij}$, and $\dot{e}_{ij}$ are the (Cartesian) components of the total, thermal, mechanical, mechanical volumetric, and deviatoric strain rate tensors, respectively. Here,