FE modelling of residual stresses and void formation observed during the growth of semicondutor layers

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Abstract

In the current approach we consider interdiffusion, lattice distortions and chemical maps corresponding the growth of SiC/Si and InGaN/GaN layers. Dislocations and free surfaces are treated as local regions for nucleation and annihilation of the vacancies transporting the mass between finite elements (FEs). In result, the interface and FE mesh are convected with the crystal lattice drift. In the constitutive modelling applied [1] the lattice distortion and the Si and vacancy molar fractions are used as independent nodal variables. Due to the climbing down of misfit dislocations the plastic distortion tensor field is taken into account in the form of additional nodal variables. This tensor field is spanned on corner nodes of the second order Lagrangian finite elements [2].

The chemo-mechanical coupling is based on the use of Vegard's law formulated alternatively in terms of Biot or Hencky strains. Due to the logarithmic strain applied in hyperelastic modelling, some transformation rule is considered for Vegard's law. This rule allowed us to eliminate artificial residual stresses yielding from incompatibility of the fields of atom fraction and plastic distortions spanned by means of the same shape functions on the corner nodes.

Keywords: residual stresses, Kirkendall effect, diffusion, mass transport, semiconductor layers, crystal growth.

1. Introduction

The interdiffusion of chemical components coupled with vacancy movement can cause the void formation driven by the chemical force and different mobility the chemical components of crystal lattice. In the case of SiC layer growth in carbonisation process of Si wafer, the higher mobility of Si atoms compared to C can result the climbing down the $\frac{\text{SiC}}{\text{Si}}$ interface and formation of voids in the substrate in some thermodynamic conditions, see Fig. 1.

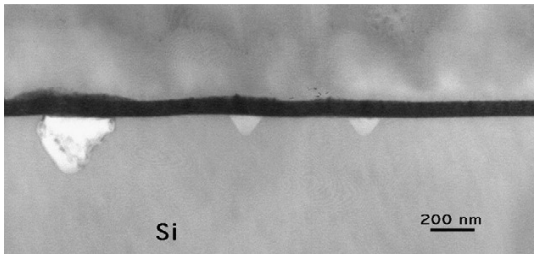

Figure 1: Voids in a silicon substrate below the SiC film (black) formed in the growth process of SiC on Si wafer, see [3].

A similar effect is observed in the case of the growth of In-rich InGaN layers on GaN substrate. The chemical force yielding from the spinodal decomposition of In-rich InGaN layer induces then the void formation on the border of metallic indium precipitations, see Fig. 2. In this talk we analyse the reasons of spurious stresses obtained during the FE calculation of stress equilibrium obtained by plastic relaxation of SiC layer grown on Si wafer.

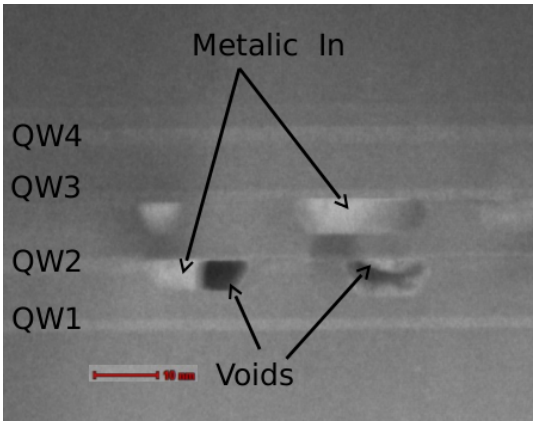

Figure 2: Voids formed in the In-reach InGaN layers. HTREM image courtesy of S. Kret.

2. Constitutive model

In the present approach, as a thermodynamic potential function we consider the following molar density of free energy

$$\psi = \frac{1}{2\widehat{c}}(\widehat{\boldsymbol{\varepsilon}} - \widehat{\boldsymbol{\varepsilon}}_{\text{ch}}) : \widehat{\mathbf{c}} : (\widehat{\boldsymbol{\varepsilon}} - \widehat{\boldsymbol{\varepsilon}}_{\text{ch}}) + \psi_{\text{ch}} \tag{1}$$

where $\widehat{c}$ is molar concentration, $\widehat{\boldsymbol{\varepsilon}}$ means the lattice strain referred to the perfect lattice of the reference material (substrate), cf. [1]. The chemo-thermal strain $\widehat{\boldsymbol{\varepsilon}}_{\text{ch}}$ and stiffness tensor $\widehat{\mathbf{c}}$ are governed by multilinear law

$$\widehat{\boldsymbol{\varepsilon}}_{\text{ch}} = \sum_{\text{i}=0}^{\text{n}-1} \widehat{\boldsymbol{\varepsilon}}_{\text{i}}\, n_{\text{i}} + \widehat{\boldsymbol{\varepsilon}}_T\, T \qquad \text{and} \qquad \widehat{\mathbf{c}} = \sum_{\text{i}=0}^{\text{n}-1} \widehat{\mathbf{c}}_{\text{i}}\, n_{\text{i}} + \widehat{\mathbf{c}}_T\, T \tag{2}$$

where $\widehat{\boldsymbol{\varepsilon}}_{\text{i}}, \widehat{\boldsymbol{\varepsilon}}_T, \widehat{\mathbf{c}}_{\text{i}}, \widehat{\mathbf{c}}_T$ are treated as material constants. By assumption, ψ_{ch} is independent of strain and depends only on the re-

maining thermodynamic variables, i.e. on $\mathsf{n}-1$ molar fractions $n_1,\cdots,n_{\mathsf{n}-1}$ and temperature T. In our case the elastic strain is identified with $\widehat{\boldsymbol{\varepsilon}}_{\mathsf{e}} \stackrel{df}{=} \widehat{\boldsymbol{\varepsilon}} - \widehat{\boldsymbol{\varepsilon}}_{\mathsf{ch}}$. The substitution of the energy function into balance equations gives the following formula for the driving forces governing the diffusion of the chemical components and vacancies

$$\widehat{\mathbf{f}}_{\mathsf{i}} = \widehat{\mathbf{a}}_{\mathsf{i}} : \widehat{\mathrm{grad}}\,\widehat{\boldsymbol{\sigma}} - \widehat{\mathrm{grad}}\,\mu_{\mathrm{ch}_{\mathsf{i}}} \tag{3}$$

where

$$\widehat{\boldsymbol{\sigma}} = \widehat{\mathbf{c}} : (\widehat{\boldsymbol{\varepsilon}} - \widehat{\boldsymbol{\varepsilon}}_{\mathrm{ch}}) \qquad \text{and} \qquad \mu_{\mathrm{ch}_{\mathsf{i}}} = \frac{\partial \psi_{\mathrm{ch}}}{\partial n_{\mathsf{i}}} \tag{4}$$

$\widehat{\mathrm{grad}}$ means the gradient operator referred to the reference crystal lattice. The constitutive equations are considered alternatively for the Hencky and Biot strain measures

$$\widehat{\boldsymbol{\varepsilon}} = \mathbf{U} - \mathbf{1} \qquad \text{or} \qquad \widehat{\boldsymbol{\varepsilon}} = \ln \mathbf{U} \tag{5}$$

where $\mathbf{U}$ is the stretch tensor of crystal lattice.

3. Finite element approach

The nonlinear matrix equation used here for simulation of the crystal growth and silicon transport to SiC layer takes form

$$\begin{bmatrix} \mathbf{C}_{\mathrm{Si}} & . \\ . & \mathbf{C}_{\mathrm{v_{Si}}} \end{bmatrix} \begin{bmatrix} \dot{\mathbf{n}}_{\mathrm{Si}} \\ \dot{\mathbf{n}}_{\mathrm{v_{Si}}} \end{bmatrix} + \mathbf{P} \begin{pmatrix} \mathbf{u} \\ \mathbf{n}_{\mathrm{Si}} \\ \mathbf{n}_{\mathrm{v_{Si}}} \\ \widehat{\boldsymbol{\beta}}_{\mathrm{pl}} \end{pmatrix} = \begin{bmatrix} \mathbf{f}_u \\ \mathbf{f}_{\mathrm{Si}} \\ \mathbf{f}_{\mathrm{v_{Si}}} \end{bmatrix} \tag{6}$$

where the nodal variables $\mathbf{u}, \mathbf{n}_{\mathrm{Si}}, \mathbf{n}_{\mathrm{v_{Si}}}, \widehat{\boldsymbol{\beta}}_{\mathrm{pl}}$ denote the displacements, the molar fraction of silicon atoms and silicon vacancies as well as a few components of the plastic distortion tensor being indispensable for plastic relaxation of SiC layer. $\mathbf{C}, \mathbf{P}$ and $\mathbf{f}$ denote the respective matrix and vectors obtained for nonlinear transient problems, cf. [4]. The distribution of Si fraction and the role of plastic distortions in relaxation of residual stresses is shown in Fig. 3-5.

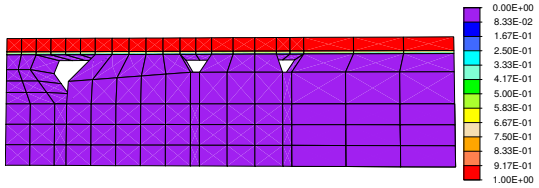

Figure 3: Si fraction assumed at the initial state

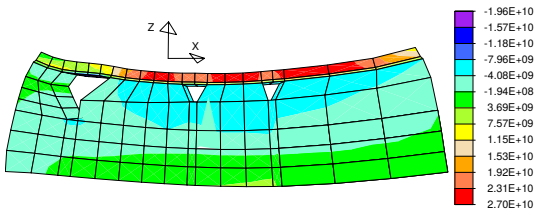

Figure 4: Residual Cauchy stresses $\boldsymbol{\sigma}_{xx}$ in SiC/Si layers induced only by chemical strains, i.e. for: $\widehat{\boldsymbol{\beta}}_{\mathrm{pl}} = \mathbf{0}$ and for free boundary conditions

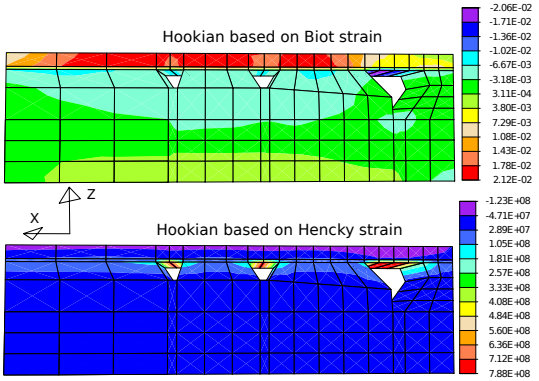

Figure 5: Spurious Cauchy stresses $\boldsymbol{\sigma}_{xx}$ in the SiC/Si layers relaxed by plastic strain for free boundary conditions

4. Conclusions

Usually, the crystal growth processes are simulated from the viewpoint of the liquid deposited on the rigid substrate. In our approach, the growth is considered from the viewpoint chemo-mechanical processes developed in the crystal lattice. The advantage of such approach is discussed.

In the talk we analyse the effect of different stress measures on the resultant residual and spurious stresses obtained in the finite element modelling. It was noted that the logarithmic strain leads to very high spurious stresses in comparison to the use of Biot strain measure. In the case of single transit finite elements situated at the interfacial zone, the mentioned approach allowed us to reduce spurious stresses in integration points from the level 10^2 MPa to 10^{-2} MPa.

References

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