Finite Element Analysis of Residual Stress Field Formed in Bimaterial GaN/AlGaN Substrates

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The last years have brought about a large development of blue light emitting laser diodes made in GaN based multilayers. The indium-rich InGaN layers deposited on GaN substrate can segregate into islands (quantum dots).
In this paper we analyse the residual stress field in a bimaterial GaN/AlGaN substrate prepared for epitaxial growth of InGaN layers. The stress field is analysed by solving a series of nonlinear finite-element boundary-value-problems [1, 2] considered for anisotropic chemo-hyperelastic material. The main source of residual stresses formed in the substrate yields from the chemo-elastic coupling (Vegard's law). The planar homogeneity of such obtained residual stress field is perturbed by the knurling-like pattern conducted on the reverse side of the substrate (on the opposite side to the epitaxial growth surface). Different finite strain measures, different sets of third-order elastic constants as well as different spatial distribution of GaN and $Al_xGa_{1-x}N$ layers in the substrate are considered in this analysis. We show how strongly the resultant pattern of stress field formed in the area of epitaxial growth depends on the assumed chemical composition, elastic model and geometrical parameters.
With respect to the wanted form of the stress-strain distribution, we consider this problem in terms of the topological optimisation of a chemo-elastic boundary-value-problem. The optimisation procedure performs a design space exploration over the geometry and chemical composition of finite element mesh. The design variables are the GaN layer thickness and the chemical composition profile. For each design instance, a full 3D hexahedral FE mesh of the multi-layer tile geometry (GaN + AlGaN layers with rounded notches) is generated, the composition distribution is assigned layer-by-layer via linear interpolation onto mesh nodes, and the weighted chemo-elastic problem is solved. After all evaluations, the best and worst designs are identified based on the minimum and maximum values of the objective function, and are subsequently visualised and exported to FEAP input files for high-fidelity verification.

Keywords. crystal growth, hyperelasticity, residual stress fields, optimisation of chemical composition

References

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