Tutorial lecture

Nonlinear finite element modelling of the residual stresses and stress induced diffusion

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The lecture is devoted to the theoretical background and practical application of the nonlinear finite element method to the analysis of chemical composition, residual stresses and stress induced diffusion in GaN based heterostructures. The lecture starts from nonlinear force-displacement behaviour of atomic bonds and constitutive equations used in the finite element modelling of residual stresses. Next, the mathematical foundations of the finite element method is discussed. A few groups of application of the method are discussed. The first one is based on the computer processing of experimental maps. This method is useful to the feed-back analysis of chemical composition and elastic distortions in chemically inhomogeneous crystalline structures with or without crystalline defects like: the quantum wells, dots, wires, rings etc. The maps extracted from HRTEM images can be used directly as the input data to the FE processing of microscopic images. The method can be also used for processing 3D maps (holography, tomography) and 2D. The maps can contain the data on chemical inhomogeneity, lattice defects, distortions, misorientations determined with the pico-nano (HRTEM) or nano-micro resolution (XRD,CBED, etc).

Another problem discussed concerns the FE simulation of the diffusion governed by two independent components of the diffusion driving force, namely: (a) the chemical force yielding from composition gradients and (b) from residual stress gradient. The forces are derived from balance equations for the energy stored in crystal lattice. The profiles of chemical compositions formed in the transient zones between layers are discussed it terms of the thermodynamic equilibrium between the mentioned forces. Some open questions as the formation of the channels on the free standing layers, the problem of the division of mass transport between the drift and diffusion, the phenomenon of interdiffusion vs. the role of transport of vacancies in the drift velocity and formation of strips, problem of the surface curvature and its influence on the surface energy and formation of dots are considered. The different theoretical and numerical approaches to the modelling of these phenomena are shown.