

## Integrated Computational Modelling of Thermochemical Surface Engineering of Stainless Steel - DTU Orbit (09/11/2017)

### Integrated Computational Modelling of Thermochemical Surface Engineering of Stainless Steel

An implicit finite difference method (FDM) based numerical model for the prediction of composition- and stress-depth profiles developing during low temperature gas nitriding (LTGN) of 316 stainless steel is presented. The essential effects governing the kinetics of composition and coupled stress evolution are taken into account in the model: concentration-dependent diffusion of nitrogen atoms, a slow surface reaction, elasto-plastic accommodation of lattice expansion and thermal and mechanical influences on thermodynamics (solubility) and diffusion kinetics. The model is one-dimensional and assumes a plane-stress mechanical state. Huge compressive stress levels and steep stress gradients have previously been suggested to have an influence on the concentration profile. The corresponding large plastic deformation that occurs in the developing case is addressed in the model by isotropic plasticity and force equilibrium. The model is used to explore the role and to assess the kinetics of the surface reaction.

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