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Stoichiometric Simulation of Nitrides and Elastic-plastic Stresses in the Course of Nitriding Process

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Strategy and results based on stoichiometry is presented for simulation on the conventional methods of evaluating volumetric dilatation due to gas nitriding and of elastic-plastic stress considering the fact that the process is limited in the very thin layer near substrate surface. One dimensional diffusion equation is solved to know the nitrogen concentration after some incubation time, where nitrogen atoms diffuse as interstitials in α-iron followed by the compound formation process. Some part of diffused nitrogen converted to form nitrides, such as γ'-Fe_4N, ε-Fe_2N and other M_xN_y. In the former case, diffused nitrogen itself enlarges the lattice parameter, and the nitrides induce the volumetric dilatation, both of which gives the intrinsic, or initial strain in the body. A conventional stress estimation method is proposed in the framework of total strain theory under the consideration that stress equilibrium equation and strain compatibility condition lead to the non-zero stress and strain in plane without shear stress and strain. If simple elastic-plastic stress-strain constitutive relation is assumed, the stress/strain profile along the depth direction is easily obtained to avoid complicated numerical calculation. Some obtained results of the simulation are compared with experimental data.

Keywords: Nitriding, Nitride compounds, Elastic-plasticity, Residual stresses,Simulation