The nitriding mathematical modelling and simulations of ferrous powder alloys

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Abstract

Mathematical modelling has been developed to improve processes control and has helped theories about complex systems to be written. Nitriding is a multivariable system that needs the convergence of efforts to allow its improvement. Computer simulation is an important tool to give a simultaneous evaluation of all variables and respective effects in the result of the process. Surface conditions have an important effect in the interaction between gases and metals. Its influence can only be studied under bidimensional and 3-D simulations. The presence of oxides and other barrier have a critical influence on the kinetic and the result of the process. Secondary reactions such precipitation and nitride layer formation also affect the process. Particularly, porosities can have an important effect by enhancing the gas permeation inside the sintered material. Depending on the variables that might be deleterious to the process, the simulations give some indications how to proceed and how to control these process variables. This work show, through simulation tools, how variables such as gas atmosphere, temperature, powder surface conditions, porosity, alloy composition will affect the final result of the nitriding process of sintered and non-sintered powders. A methodology was developed using numerical methods and systemic algorithms.

Introduction

Nitriding is a important process to improve surface properties of a steel. There are various kinds and variations from that which could let be difficult a general approach for mathematical models. In fact, nitriding is a typical metal/ gas reaction where exist surface reaction phenomena, phase transformations, mass transport through the bulk material and so one. The systematisation of those process can allow to a effective and helpful simulation tool.
Theorical concepts of nitriding process were based upon a joining of Fe-N diagram and diffusion process [1-5]. This approach is useful to a theorical treatment of experimental data from nitriding of pure iron. Instead a mathematical model blow up from that approach, simulations "a priori" are difficult to foresee or fit experiments from nitring of steels.
Typical diffusion curves obtained from solutions of Fick's equations [6] are not good fittings to experimental curves, as schematically showed in Fig 1. This lack between experimental works and theory shows that a more complex phenomena are present on nitring. Some conceptual efforts were made by Jack and co-workers [7] in earlier works. Basically, this author pay attention to microstuctural effects, such as precipitation of nitrides, solid solution and diffusion questions, on results of diffusion pattern of nitrogen. But there were nothing in mathematical approaches to simulation tools.