11th International Conference
on Advanced Materials
Rio de Janeiro Brazil
September 20 - 25
ICAM2009

HRTEM and Molecular Simulation Analysis of ε - $Fe_{2-3}N$ AND γ' – Fe_4N Nitrides

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Abstract – Both high resolution transmission electron microscopy (HRTEM) and molecular simulation techniques were applied to optimize the analysis of the nitrides formed on the top surface in samples nitrided by post-discharge microwave. The theoretical calculations were made over an Indigo2 SGI workstation whit a R10000 processor and using the Cerius^2 software by MSI. The experimental analyses were carried out in a FEG-HREM PHILIPS TECNAI F20. The results showed that the characteristic morphology of the γ' – Fe_4N crystal is associate at regulate squared faces in the [0 0 1] orientation and it growth whit planes surfaces at 45 degrees and the ε - $Fe_{2-3}N$ crystal is associated at regulate hexagonal faces in the [0 0 1] orientation and it growth whit planes surfaces at 30 degrees between its planes respectively.

The nitrided layers have been studied by several characterization techniques [1]. However these studies have been rarely accompanied by theoretical analysis. Molecular simulation techniques have gained strength amongst the scientific community during the last two decades, for molecular and crystal systems, and by classical and quantum mechanism approximations. Computational material science can be used as a virtual laboratory, where the electronic structure, charge distribution and atomic configuration, are analyzed by quantum mechanics calculations, using both semi-empirical and density functional theory based approaches, that allow the identifications of reactions conditions, molecular selectivity and predict macroscopic properties. In this sense, it is important to either confirm or to refine the models and the corresponding predictions through a comparison between theoretical and experimental data. This fact provides an easier interpretation and identification of small details from the materials. In particular, the high resolution transmission electron microscopy (HRTEM) images interpretation could be really complicated, especially when more than one crystalline matrix exists or when the particles are nanometric and any tilting or focusing changes could lead to a misinterpretation of the image. In this work, we report the analysis made by X-ray diffraction to determine the crystalline phase formed during 15 minutes of treatment by post-discharge method, while HRTEM was used to determine the structure and composition of local arrangements of crystalline grains and nanoparticles. Concerning the analytical data, we used molecular and HRTEM simulation tools for a better understanding and a well-supported interpretation of the experimental results.

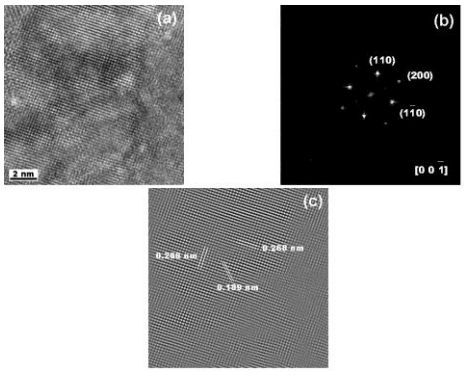

Figure 1: HRTEM image from (a) γ' – Fe_4N phase at the surface layer, (b) the FFT in the [0 0 1] axes and (c) the processed image with distances between parallel atomic planes of 0.268 nm and 0.219 nm

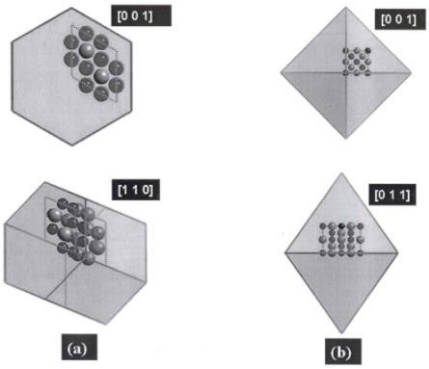

Figure 2: Calculated morphology for (a) ε - $Fe_{2-3}N$ in [0 0 1] and [1 1 0] orientation and (b) γ' – Fe_4N in [0 0 1] and [0 1 1] orientation.

(1) A. Medina-Flores, J. Oseguera, P. Santiago, J. A. Ascencio. Structural Analysis of AISI-SAE 4140 Steel Nitrided by Post-Discharge Microwave. Surf. & Coat. Technol. 188-189 (2004) pp. 7-12.