

Simulation molecular of the ϵ - $\text{Fe}_{2.3}\text{N}$ nitride obtained by HRTEM from a low carbon steel nitrided

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The nitriding treatments have been introduced to improvement the properties in iron and alloys. The nitriding is a termo-chemical process that produces a profile concentration of N from the top surface toward inner of the material. This profile produces nitrides formed by different elements whit affinity whit the N to form nitrides. The nitriding involve diffusion of N in the metal at temperatures close and below of the eutectoid transformation point (580 °C) in the Fe-N o Fe-N-C systems. The nitriding treatment can be carry out by different treatments: Solid, liquid, gas, plasma and post-discharge microwave.

In the nitriding treatment by post-discharge micro-wave, the reactive atmosphere is composed of neutral excited species. In this process, the neutral species excited and the solid produces higher kinetics the growing of nitrides, which are faster compared whit the conventional process [1-2]. In the surface nitrogen concentration rapidly reach values associated with the formation of ϵ - $\text{Fe}_{2.3}\text{N}$ phases. Typically, iron and steel nitriding temperatures are close and below the eutectoid transformation point. Nitride layer growing kinetics is associated to the nitrogen diffusion rate through this layer. The nitriding samples were analyzed in a FEG-TEM Tecnai F20 at 200 Kv. Molecular techniques simulation were also applied to optimize the microstructural analysis, the studies were carried out using the software Cerius² version 3.0, the theory analysis were made in a work station Indigo2 SGI whit a R10000 processor. The samples were prepared by the conventional grinding method. The figure 1a show a TEM micrograph of the ϵ - $\text{Fe}_{2.3}\text{N}$ nitride, whit an interatomic distance of 0.219 nm, figure 1b show the fast fourier transform of the nitride in the $[1, \bar{1}, 2, 0]$ direction, figure 1c show the crystal model in the $[1, \bar{1}, 2, 0]$ direction the figure 1d show the morphology in the $[1, \bar{1}, 2, 0]$ direction and the figure 1e show the HRTEM image simulated of the ϵ - $\text{Fe}_{2.3}\text{N}$ nitride in the $[1, \bar{1}, 2, 0]$ direction. Frequently, the surface compound zone is also formed on top of the diffusion zone, with thickness in the micron range. In the diffusion zone, the microstructure is changed by the introduction of single interstitial N atoms in solid solution and when solubility limit is reached, very fine coherent precipitates are formed. The hardness is only slightly changed by the nitrogen in solid solution, while the hardness increases substantially when the nitride precipitates form, depending on the nitride-forming alloying elements. Molecular simulation techniques are bigger tools that let us make an analysis between the experimental and theory results, let it an improvement of the properties of the materials.

References

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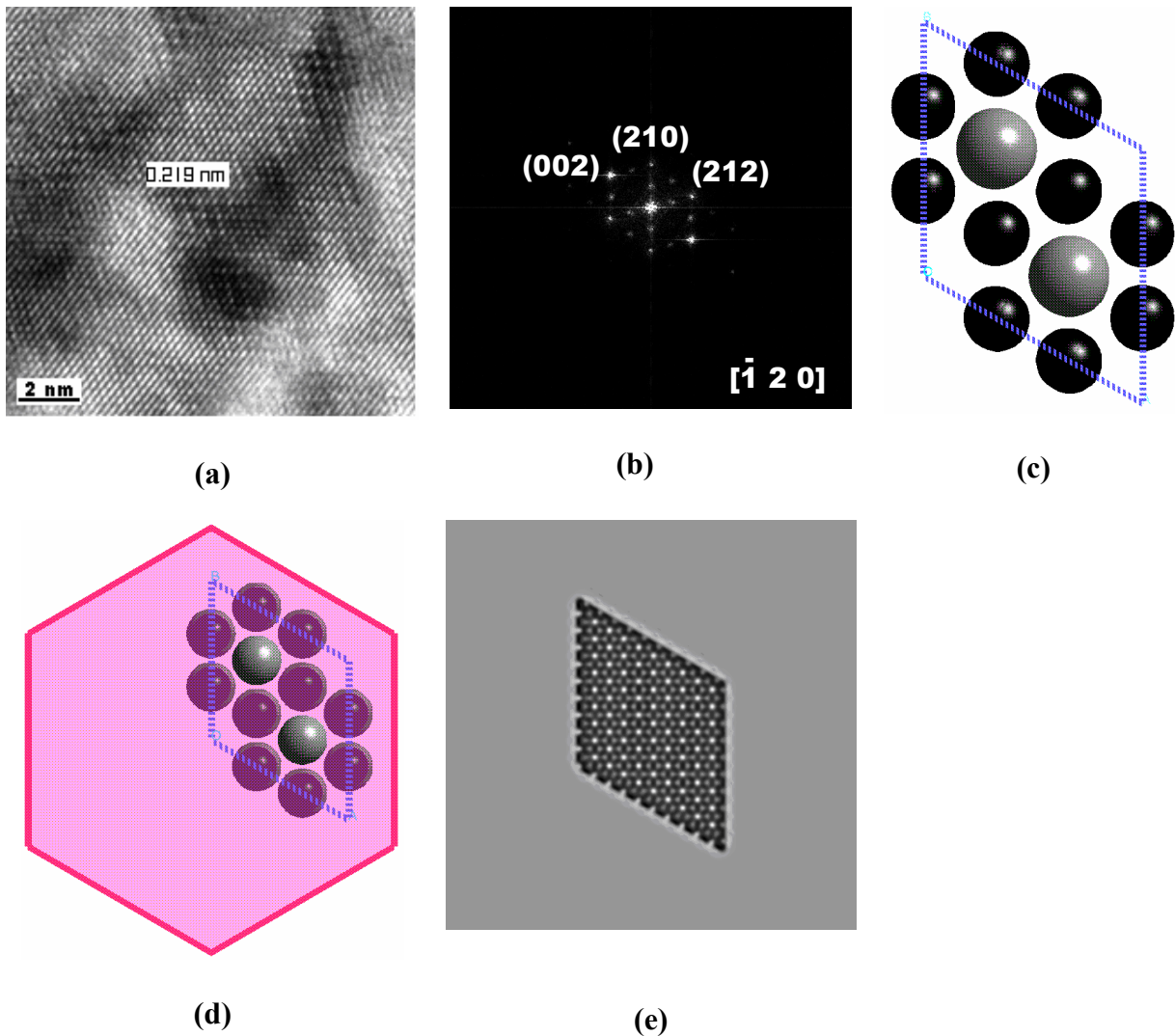


Figure 1. (a) HRTEM image of the ϵ - $\text{Fe}_{2.3}\text{N}$ nitride showing an interatomic distance of 0.219 nm. (b) Fast fourier transform in the $[1, \bar{1}, 2, 0]$ direction. (c) Crystal model of the ϵ - $\text{Fe}_{2.3}\text{N}$ in the $[1, \bar{1}, 2, 0]$ orientation. (d) Morphology of the ϵ - $\text{Fe}_{2.3}\text{N}$ in the $[1, \bar{1}, 2, 0]$ orientation. (e) HRTEM simulated of the ϵ - $\text{Fe}_{2.3}\text{N}$ in the $[1, \bar{1}, 2, 0]$ orientation.