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Diffusion of non-magnetic impurities in ferromagnetic α-Fe

R.A. Pérez[1*]

(1) Dto. de Materiales, Comisión Nacional de Energía Atómica (CNEA), Bs As, Argentina., e-mail: rodperez@cnea.gov.ar
* Corresponding author.

Abstract – Diffusion of several non-magnetic impurities in ferromagnetic α-Fe was measured. The same behaviour was found, consisting in a downward curvature in the Arrhenius plot doe to a ferromagnetic influence on the diffusion process. Ab initio calculations were performed in order to model such effect.

Substitutional and self-diffusion in α-Fe show a break in their Arrhenius plot at the Curie temperature, T_C, follow, at lower temperatures, by a downward curvature which is ascribed to the effect of ferromagnetic on the diffusion process [1]. In these work the measurement of diffusion in α-Fe of several non-magnetic elements, all constituents of different kind of steel alloys, like Sb, Sn, As, Ni, and W, is presented. A common behaviour was found.

Measurements were performed combining Rutherford Backscattering Spectrometry (RBS), RBS with Heavy Ions (HIRBS) and Secondary Ion Mass Spectrometry SIMS techniques.

The ferromagnetic alignment of Fe spins induces an increase in the activation energy Q^f respect to the paramagnetic situation; this increase is different for different diffusers when they are magnetic, like Co or Cr, but it was found constant, within the experimental error, for all the non magnetic impurities here studied.

Ab-initio calculations were also performed using WIEN2k algorithm, in order to model and understand such behaviour. It was found that the magnetic interaction among the magnetic spin of the Fe atoms involved in the diffusion jump are the only responsible for the activation energy increment when the diffuser is non-magnetic, whereas and additional term including the interaction between the diffuser spin and the Fe spins has to be consider for magnetic diffusers.

[1] K.Hirano, and Y.Iijima Defect and Diffusion Forum **66-69** 1039 (1989)