# Diffusion simulation of Cr-Fe bcc systems at atomic level using a random walk algorithm

*I. San Sebastian*[1], *J. Aldazabal*[1], *C. Capdevila*[2], *C. Garcia-Mateo*[2]

[1] *CEIT and Tecnun (University of Navarra), Paseo Manuel de Lardizábal 15, 20018 San Sebastián, Spain*
[2] *MATERALIA Research Group. Department of Physical Metallurgy, Centro Nacional de Investigaciones Metalúrgicas (CENIM-CSIC), Avda. Gregorio del Amo 8, E-28040 Madrid, Spain*

*jaldazabal@ceit.es*

From a "macroscopic" point of view, material composition is assumed to vary smoothly along its microstructure. A closer look reveals that, at the atomic level, the material composition does not change so smoothly. Single atoms jump randomly along the crystal lattice due to their thermal energy. These random jumps create sporadic zones of the crystal with higher concentration of certain elements, and they are responsible for many phenomena, such as spinodal decomposition, segregation, precipitation, Ostwald ripening… This work simulates the diffusion of Cr and Fe in a Fe-Cr system at atomic level. Simulated temperatures are in the range of 650-750 K, where the atomic structure of both isolated compounds are bcc.

The full 3D model developed takes into account for the random jumps of substitutional Cr through the Fe-bcc lattice sites, neglecting the system vacancies at this temperature [1]. The model was applied to simulate the evolution of a flat composition front in a prismatic domain. This domain was divided into small prisms to run simulation in a cluster of computers in parallel. The cluster used consist of 24 Pentium IV processors at 2.6 GHz and requiring about 13 GB of physical memory [2].

A set of simulations was run to study the relationship between the atomic jump rate and the macroscopic-continuum diffusion coefficient. This study was performed using continuum calculations using Dictra™ software [3]. Figure 1 shows concentration profiles obtained by the proposed model after 3761 jumps of each Cr atom and Dictra results for a diffusion time of 3072 hours at 748 K.

Different set of simulations was run to study the relationship between jump rate and temperature. Results of this part are represented in figure 2. These results were fitted to an Arrhenius type equation, allowing for the determination of the Cr atomic jump activation energy at 306 kJ/mol, which is in good agreement to the empirical value of Cr diffusion in Fe-bcc, 250 kJ/mol [4].

The results obtained by means of the model will be useful to study at atomic scale phenomena, such as the Cr segregation in Fe based alloys, or the spinodal decomposition that takes place in these materials at low temperatures.

**References:**

[1] J. Aldazabal, C. Garcia-Mateo, *Materials Science Forum*, **500-501** (2005) 719-726.
[2] M. Creel, http://idea.uab.es/mcreel/ParallelKnoppix (Online March 2007).
[3] Dictra User's guide (Dept. Of Materials Science and Engineering) Royal Institute of Technology, Sweden (1998) 63-71.
[4] A.W. Bowen, G.M. Leak, *Metallurgical Transactions*, **1** (1970) 1695-1700

**Figures:**

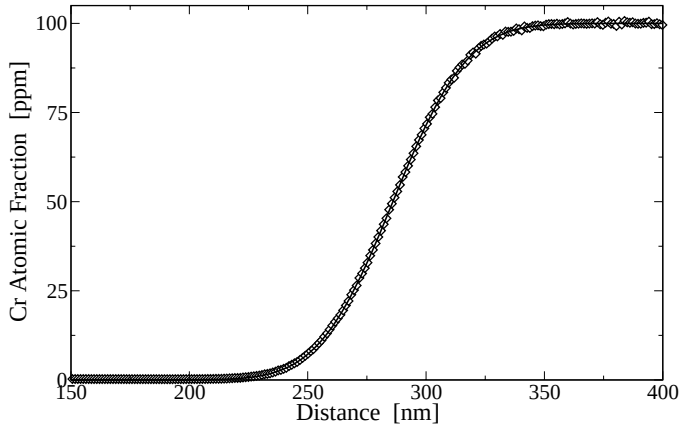


**Figure 1:** Comparison of concentration profiles obtained using proposed model after 3761 jumps of each Cr atom and continuum Dictra calculation for 3072 hours@748 K.

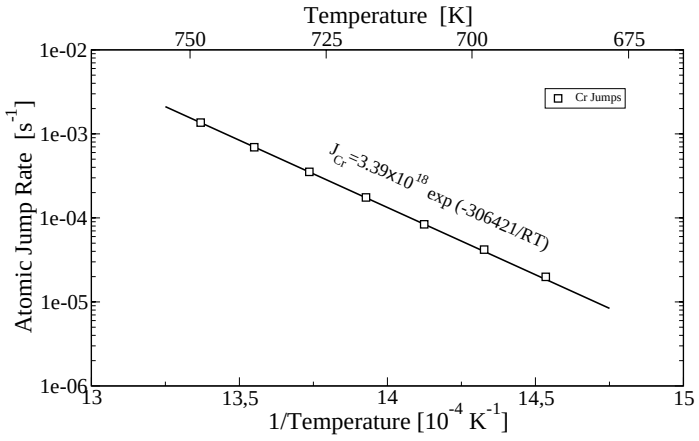


**Figure 2:** Simulated atomic jump rate of Cr in a pure bcc Fe matrix at different temperatures and its Arrhenius fitting.