Atomic scale simulation of Carbon electromigration in Iron

Detailed description of the framework:

Electromigration is an electric field induced mass transfer in solids. To describe this phenomenon, the model considers that each specie has an equivalent electric charge. This project has two main objectives: determine the physical phenomena that lead to this equivalent electric charge in order to simulate electromigration at the atomic scale. In this project, we focus on the electromigration of Carbon in Iron since the production of steel is the largest metal production in the world. Iron is used in a wide range of fields such as aerospace and automobiles, but it needs to be strengthened before it is used in these fields. There are many ways to strengthen it, such as work hardening, solid solution strengthening, and grain boundary strengthening. The diffusion of Carbon atoms in Iron is related to solid solution strengthening. Since the interstitial diffusion of Carbon atoms affects the reaction rate of phase transformation of steel, the properties of Iron are affected by the Carbon inside the Iron. Until now, the main driving force for carbon diffusion was considered to be transfer by heat, but in recent years, in the Spark Plasma Sintering method, carbon diffusion by an electric field has attracted a great deal of attention. However, although the study of Carbon diffusion in Iron by thermal diffusion has been widely conducted, the study of Carbon diffusion under electric current has not been sufficiently conducted especially when C diffusion induced by the electric field leads to the allotropic phase transformation (from ferrite to austenite).

When an electric current flows through a solid, atoms are submitted to forces which induce mass transfer. This phenomenon, named electromigration, has been studied to increase the life duration of metallic connectors in microelectronic devices. In metallurgy, Joule heating is more often used during material processing in order to increase productivity and decrease energy consumption. However, compared to classical heating (radiative and or convective heating) the influence of the electric current leads to different material microstructure and thus mechanical properties. It is then important to understand and model electromigration. One of the key points of the model is the determination of the equivalent electric charge of the atoms.

The common model of the electromigration of C in Fe is to consider C as an ion in the Fe lattice. The equivalent charge Z* of the C ion has experimentally been determined [1-5] by comparison of the experimental C concentration with theoretical prediction accounting for the presence of the electric field in the sample. In the mentioned model, the C ions are submitted to the classical thermal diffusion and to a drift velocity induced by the electric field: $V_d = \frac{Z^* EDe}{k_b T}$ (1) [1].
The reported values of the equivalent charge of C may vary from +3 to +15 depending on the temperature level, the current density and the solid phase. These values of equivalent charge are nonrealistic considering that C atom has only 6 electrons. This points out the need for a physical understanding of the phenomenon. We intend to get a better understanding of the variation of Z* using ab initio calculations.

1 In equation (1): *E* is the electric field, *D* the diffusion coefficient, *e* the coulomb charge, k_b the Boltzmann constant and *T* the temperature

As carbon diffuses into iron, C concentration gradients may appear leading to solid phase change of iron (from ferrite to austenite) and then microstructure change. Our goal is to use ab initio calculation results in order to simulate electromigration of C into Fe at the atomic scale, using molecular dynamics simulations, and study the influence of the electric current on the solid phase change induced by C electromigration.

This project is part of a collaboration between MATEIS (INSA de Lyon), ILM (University Claude Bernard Lyon 1) and IFS (Tohoku University).

Each part has abilities in different fields the allow to address the problem that has to be studied:

Patrice Chantrenne, Professor at MATEIS laboratory, carry out experiments to study electromigration in steels. He also does molecular dynamics simulations.

Christophe Adessi (http://ilm-perso.univ-lyon1.fr/~cadessi/), Assistant Professor at ILM (https://ilm.univ-lyon1.fr/) is a specialist of *ab initio* simulations and quantum transport calculations.

Takashi Tokumasu, (http://www.ifs.tohoku.ac.jp/nanoint/eng/member/tokumasu/index.html), Professor at IFS (http://www.ifs.tohoku.ac.jp/eng/), leads research in mass transfer at atomic scale using molecular dynamics.

Work program and expected schedule:

To resume, to get a predictive model for C diffusion in iron submitted to an electric field, it is important to know the value of the equivalent charge of the C atom in a Fe lattice. The overall objectives of the project are:
a/ The physical origin of this surprising large equivalent charge, Z*, is still unknown: we intend to get a better understanding of the variation of Z* as function of the electric field, using *ab initio* calculations. One expects to determine the equivalent electric charge Z* from the forces exerted on the C atoms under a DC field. Both ferrite and austenite structures will be investigated and compared to the experimental values reported in the literature.
Duration: 6 months for Training with DFT codes (SIESTA, QE, VASP …) and calculations implying electric field.
6 months for the determination of the effective charge Z function of the current density.*

b/ Molecular Dynamics (MD) simulations will be used to simulate C electromigration in Fe at the atomic scale. The goal is to compare the drift velocity obtained by MD with the one predicted by the equation (1). From the value of Z* obtained in part **a**/, determination of the drift velocity using MD simulation function of the current density and the temperature level in the two solid phases of iron.
Duration: 6 months starting with MD training and then application to the simulations.

c/ C diffusion may locally induce a C concentration increase, leading to a solid phase change in Fe : our goal is to simulate this phenomenon at the atomic scale in order to investigate the role of the electric field on the solid phase change in Fe. The interatomic potentials used in

MD may not lead to realistic prediction for phase change. In such case, we may attend to use first principle MD to study solid phase change in Fe induces by C diffusion.

Duration: 1 year

Papers and PhD report: *6 months*

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