DFG-Projekt Schm 746/101-1

Multiscale simulation of the Fe-Cu-Ni-Mn energy system: towards structural optimization of the precipitates distribution

Project start: 01.06.2010
Project end: 31.05.2012

Goals

Copper, Nickel and Manganese allowed steels are widely used in power stations as material for pipelines and pressure vessels. These alloys permit higher hardness and tensile stress at the high operational temperatures of power stations, which vary between 300°C and 450°C. After years of operation hardening together with an decrease of ductility occur.

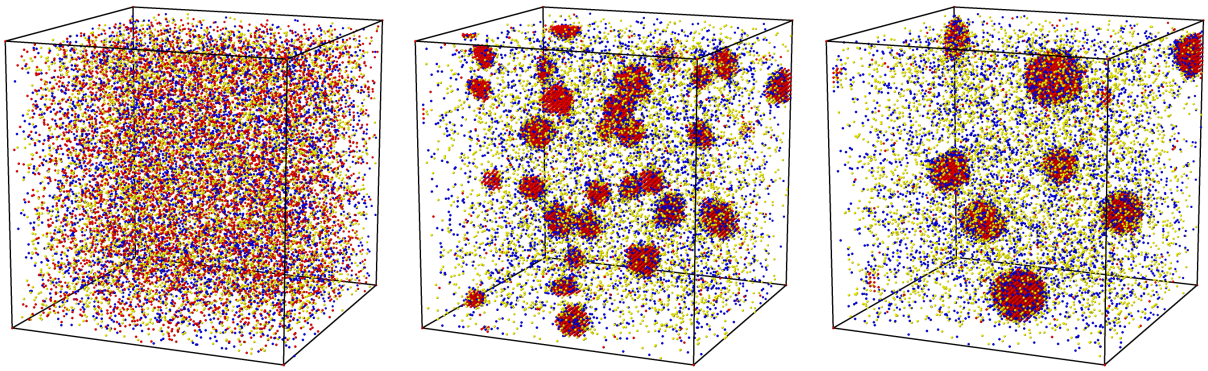
The goal of this project is a realistic simulation of copper-rich clusters (precipitates) towards the optimization of their distribution for the energy system Fe-Cu-Ni-Mn. The clusters formation and growth will be investigated in detail using Monte-Carlo simulations for the relevant temperatures and alloy concentrations. In addition, phase-field simulations developed at the Institute of Materials and Processes of the Karlsruhe University of Applied Sciences (IZBS) will provide a continuum mechanical description of the involved processes. Based on this, the influence of the alloy elements on the cluster formation as individual units as well as on their mutual interactions shall be better understood. The planned simulations shall give insight into the temporal evolution of the clusters radii and distribution of inter-cluster separations as well as their chemical composition. The aim of the simulations is to obtain clues for the improvement of the material properties of Copper-, Nickel-, and Manganese-alloyed steels.

Material

The simulations will be carried out for the systems Fe-Cu, Fe-Cu-Ni, Fe-Cu-Mn und Fe-Cu-Ni-Mn, with the aim of exploring the influence of the alloy elements on the cluster formation. The temperature should range between 360 and 500°C in order to be able to compare simulations with experimental results. The Cu concentration should be 0.65%, 1.00%, and 1.50% respectively; the Ni concentration 1.3% and the Mn concentration 0.95%.

Methods

The main idea of this simulation method is based in a physical description of the position exhange between a vacancy and next neighbor lattice atoms. This kind of thermal activated diffusion processes can be simulated in detail by means of a direct Monte-Carlo algorithm. Migration energies and attempt frequencies will be obtained from recent experimental diffusion data and ab initio computations and then used as input parameters for the Monte-Carlo simulations. In the Fe-Cu system, a better understanding of the dependence of the cluster form and size should be attained. For the systems Fe-Cu-Ni, Fe-Cu-Mn and Fe-Cu-Ni-Mn the influence of the alloy elements Ni and Mn respectively on the clusters form and their chemical composition shall be investigated. The interfacial energies between a cluster and the surrounding matrix will be used as input parameter for the simulations developed in the IZBS in Karlsruhe. This will be accomplished with the software VASP (Vienna ab-initio simulation package), which performs ab initio computations based on the Density Functional Theory (DTF).



(a) T=500°C, t=0, $\bar{R}$=0 (b) t=8.8 hours, $\bar{R}$=1nm (c) t=79 hours, $\bar{R}$=1.57nm

Snapshots of the Monte-Carlo simulation for the system Fe-Cu-Ni-Mn- (Cu 1.5 wt% - Ni 1.3 wt% - Mn 0.95 wt%) . (a) Starting with a uniformily random distribution of Cu-(red), Ni-(yellow), and Mn-(blue) alloy elements, precipitates are formed. Fe-Atoms are not depicted. (b) After 8.8 hours, precipitates with average radius R=1nm are formed. For further simulation stages, larger precitates grow incorporating smaller ones (the so called Otswald ripening). (c) After 79 hours the average radius has grown to R=1.57 nm.

The classical theory of the cluster growth divide the process in stages: cluster formation, growth, and Otswald ripening (coarsening of the larger clusters at expense of the smaller). The temporal evolution of the mean cluster radius and the cluster radii distributions should be investigated with the help of the Monte-Carlo simulations. The resulting cluster radii distributions and the coarsening rates should be compared with those from the continuous mechanical theory of Lifshitz, Slyozov und Wagner (LSW).

In the frame of the current joint work with the Fraunhofer Institut für Zerstörungsfreie Prüfverfahren (IZFP) in Saarbrücken, the results of the Monte-Carlo and phase-field simulations will be compared with corresponding experiments. In order of obtain a realistic image of the lattice dynamics, the relaxations of the atomic bindings and the (in-)coherence of the Cu and Cu-Ni precipitates dependence of the cluster size will be investigated with help of molecular dynamics simulations.

Partner

This project will be conducted in a close collaboration with the Institute of Materials and Processes of the Karlsruhe University of Applied Sciences.

Acknowlegment

The research will be sponsored by the Deutschen Forschungsgemeinschaft (DFG) under the number 746/101-1. We are grateful to the DFG for the financial support.

Contact Person

Dr.-Ing. Peter Binkele
Tel.: +49 / 711 685-62595 / E-mail: peter.binkele@imwf.uni-stuttgart.de

Dr. rer. nat Alejandro Mora
Tel.: +49 / 711 685-62701 / E-mail: alejandro.mora@imwf.uni-stuttgart.de