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Investigación en transformaciones controladas por difusión en aceros resistentes al creep y gradientes en carburos cementados: Resultados experimentales y simulaciones por DICTRA

Investigations on diffusion – controlled transformations in creep resistant steels and graded cemented carbides: Experimental and DICTRA simulations

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Executive Summary

The objective of this work was to simulate diffusion-controlled transformations on engineering alloys designed by the author and his colleagues. The main challenge of the work is to adapt the existing DICTRA models to the experimental processing and working conditions investigated, as well as to find the adequate boundary conditions for the description of the diffusion-controlled transformations governing the microstructure formation and evolution, in order to obtain reliable simulation results. The simulations were compared with experimental results of the microstructure evolution by scanning electron microscopy and scanning transmission electron microscopy (STEM).

Two groups of materials were investigated. The first group was 9-12% Cr heat resistant alloys. These alloys are particularly interesting because the microstructure evolves during working conditions. Different compositions were designed in order to form different kinds and amounts of precipitates. For the designed 9-12% Cr creep steels the coarsening of MX and $M_{23}C_6$ particles was modeled by applying the coarsening model implemented in DICTRA. The cell method of DICTRA was applied to investigate the kinetics of the Laves phase growth on 9-12% Cr alloys. The particular objectives of these investigations were: a) to determine the coarsening rate of precipitates, b) to investigate the influence of alloying element on the growth rate of the Laves phase, c) to determine the influence of the $M_{23}C_6$ formation on the growth kinetics of the Laves phase, d) to determine the growth mechanism at the interface of the Laves phase (i.e. up-hill diffusion), e) to investigate the effect of the cell size on the simulation kinetics of Laves phase.

The second group of materials was cemented carbides. They are used as cutting tools or wear parts in the automotive, aircraft and mining industry among others. The wear performance of cemented carbides (hardmetals and cermets) can be largely improved by applying wear resistant thin films by (CVD). The production of a graded outer-surface layer is necessary in order to ensure good adhesion of the coating to the cemented carbide and to avoid crack propagation. The formation of the graded outer-layer is a diffusion-controlled process. DICTRA calculations were carried out to model the formation of the

graded layers. The particular objectives of the investigations were: a) to simulate the growth kinetics of the graded layer for different periods of sintering time, b) to observe the influence of the mobility values on the kinetics of layer formation, c) to adjust the mobilities of the diffusing elements in order to have a good fitting with the experimental results.