Atomic-scale modeling of point defects, phase stability, and the formation of Z phases CrMN (M=V, Nb, Ta) in steel

Daniel F. Urban[1] and Christian Elsässer[1,2]

[1] *Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany*
[2] *Freiburg Materials Research Center (FMF), Albert Ludwig University of Freiburg, Germany*

The challenge of raising the steam inlet temperature of fossil-fired power plants calls for creep-resistant steels with a Cr content higher than 9% in order to achieve sufficient corrosion and oxidation resistance. However, it has been observed during long-time power-plant operation that in 11-12% Cr ferritic-martensitic creep-resistant steels strengthened by fine-grained (V,Nb)N particles, precipitation of thermodynamically stable Z-phase particles, CrMN (M=V, Nb, Ta), is unavoidable and detrimental. Usually, Z-phase particles are coarse-grained and brittle, and they grow at the expense of the desired, beneficial (V,Nb)N particles. A promising solution to this problem is provided by the idea to exploit the Z phase as a thermodynamically stable mechanical strengthening agent. Hence the challenge is to control the precipitation of the Z phase such that fine-grained and long-time stable particles are formed.

We present atomistic simulations, based on density function theory calculations, which reveal the essential thermodynamic processes and kinetic mechanisms underlying the formation of ternary Z phases from binary metal-nitride (MN) particles in Cr-containing steel. The scenario that evolves (figure 1) consists of the diffusion of Cr atoms into MN particles with the rocksalt structure and the subsequent clustering of Cr atoms in a layered arrangement which finally results in the transformation of the MN particles to Z-phase particles with multilayer [Cr/MN] structure. The energetic stability of Z phases with respect to related compounds as well as the thermodynamics and kinetics of atomic defects in MN involved in the Z-phase formation are investigated.

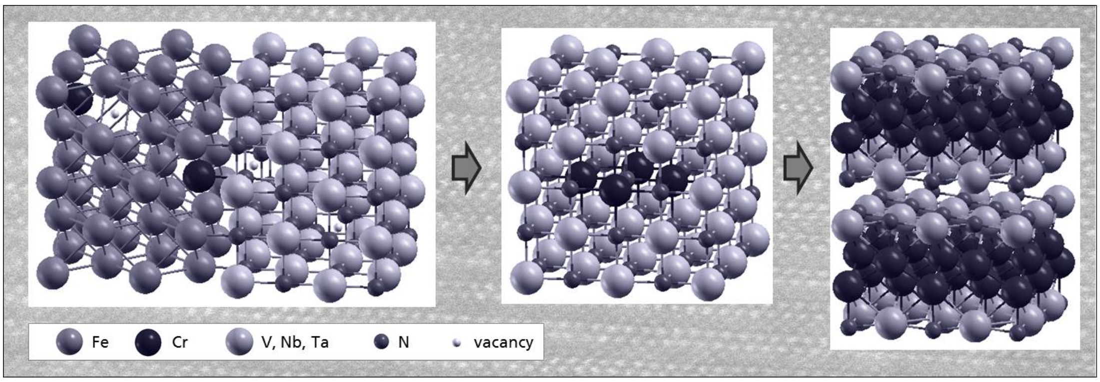

Figure 1: Formation of a Z phase CrMN from MN in Cr-containing steel: Cr atoms diffuse from the Fe matrix into the MN particle (left), they agglomerate to planar Cr clusters (middle), and these grow to extended Cr layers in MN, forming the multilayered [Cr/MN] structure (right) of the Z phase.

This work is part of the research project Z-Ultra (www.z-ultra.eu) funded by the European Commission (FP7-NMP-2012-2.2-3, Grant Agreement No. 309916).