

## MM 54: Invited talk Urban

Time: Thursday 9:30–10:00

Location: BAR 205

**Invited Talk** MM 54.1 Thu 9:30 BAR 205  
**Revealing the mechanism of Z-phase formation in 12% Cr ferritic-martensitic steels** — DANIEL F. URBAN and CHRISTIAN ELSÄSSER — Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

The objective of increasing the efficiency of fossil-fired power plants by raising the steam inlet temperature calls for ferritic-martensitic creep-resistant steels with a Cr content higher than 9% in order to achieve sufficient corrosion and oxidation resistance. However, it has been found that for 11-12% Cr steels strengthened by fine (V,Nb)N particles, these precipitates transform during long-term service into coarse, thermodynamically more stable Z-phase particles, CrMN (M=V,Nb,Ta),

that deteriorate the steels mechanical behavior. We present extensive atomistic simulations, using density functional theory, that shed light on the essential mechanisms underlying the formation of the detrimental Z-phases and help to understand their respective dependencies. Our results reveal that the Z-phase transformation proceeds via diffusion of Cr atoms into the MN particles and their subsequent clustering in a layered arrangement of the Z-phase. We systematically scan the configuration space of various intermediate structures by varying their morphology, stoichiometry and point defect concentration. Our results support the ongoing experimental efforts to control the precipitation of the Z-phase through appropriate microstructural engineering and to exploit a fine distribution of the Z-phase itself as strengthening agent in the newly developed 12% Cr steel.