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Interplay between alloying and tramp element effects on temper embrittlement in bcc iron: DFT and thermodynamic insights

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The details of the temper embrittlement mechanism in steels caused by impurities are unknown. Especially from an atomistic point of view, there are still open questions regarding their interactions with alloying elements such as Ni, Cr, and Mo. Therefore, we used density functional theory to investigate the segregation and co-segregation behavior and the resulting influence on the cohesion of three representative tilt grain boundaries in iron. The results are implemented in a multi-site and multi-component kinetic and thermodynamic model for grain boundary segregation, to gain insights into the temporal and final grain boundary coverage. Our results show that the segregation tendency of As, Sb, and Sn is stronger than that of the alloying elements and significantly mitigates the grain boundary cohesion. Depending on the GB type, interactions between Sb and Sn vary from negligible to strongly attractive, which increases the likelihood of co-segregation. The cohesion-weakening effect is further amplified when elements such as Sb, Sn, and As co-segregate, compared to their individual segregation. In contrast, the co-segregation of Ni and Cr does not significantly increase the enrichment of impurities at grain boundaries, and their impact on cohesion is found to be negligible. The ability of Mo to mitigate reversible temper embrittlement is primarily attributed to its cohesion-enhancing effect and its capability to repel tramp elements from GBs, rather than scavenging them within the bulk, as suggested by previous literature.

Speaker Country

Austria

Primary author: Mr AMIN, Sakic (Montanuniversität Leoben, PHD student at the Department of Materials Science)

Co-authors: Prof. SCHNITZER, Ronald (Christian Doppler Laboratory for Knowledge-based Design of Advanced Steels, Department of Materials Science, Montanuniversität Leoben); Dr HOLEC, David (Christian Doppler Laboratory for Knowledge-based Design of Advanced Steels, Department of Materials Science, Montanuniversität Leoben)

Presenter: Mr AMIN, Sakic (Montanuniversität Leoben, PHD student at the Department of Materials Science)

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