Poulumi Dey

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Research topics:
Ab initio based study of coherent microstructure, Phase stability, Phase boundary, Precipitation kinetics, Hydrogen embrittlement

Chemo-mechanical coupling at coherent interfaces

Research activities:

The dispersion of nano-sized coherent precipitates in a solid solution is an effective way to design materials with outstanding mechanical properties. The lattice mismatch between the precipitates and the matrix determines the local chemical equilibrium at the coherent interfaces, the distribution of the nano-precipitates, stability against coarsening and the interaction with dislocations under an applied stress. Powerful metrological techniques exist e.g. scanning transmission electron microscopy (STEM) and atom probe tomography (APT) which are capable of resolving atomic scale compositional fluctuations at interfaces. However, in spite of the enormous progress made over the past decades in improving their spatial and elemental resolution, both techniques suffer from limitations that restrict their capabilities to resolve structural and compositional features individually.

In a recent work [1], we demonstrated a novel nano-metrological approach correlating STEM, APT and density functional theory (DFT) to understand the impact of the coherency strain on the C partitioning in an austenitic Fe matrix strengthened by coherent κ carbide precipitates. Fig. 1a shows an overview high angle annular dark-field (HAADF) STEM image and the corresponding 3D-APT reconstruction of C. It is found that the Fe matrix is tetragonally strained in nanometer sized (narrow) matrix

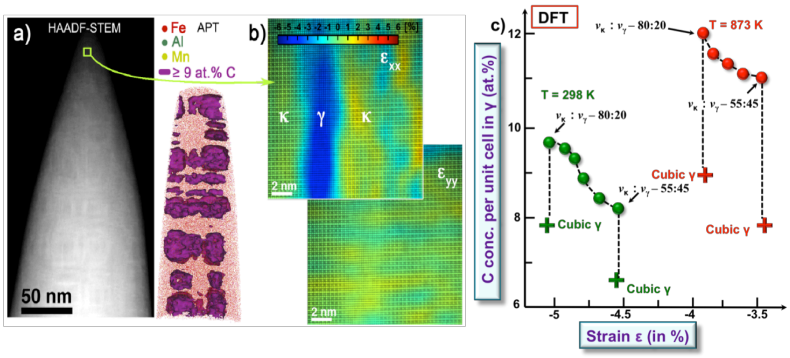

Fig. 1 a) HAADF-STEM image and corresponding APT reconstruction of the same specimen b) Atomically resolved HAADF-STEM images and corresponding strain maps c) C concentration in Fe-matrix as a function of tetragonal strain obtained from DFT

channels as can be seen from quantitative HAADF-STEM images in Fig. 1b. APT determines the concentration of C in γ-Fe around the precipitates to be approx. 5 at.%, but compositional differences in the broad and narrow γ-Fe channels are not detectable. In this regard, the DFT calculations establish that an increasing tetragonal strain leads to an increase in C concentration. Such an observation is capable of explaining the experimentally observed broad C concentration gradient across the interface, since the first atomic layers of γ-Fe in proximity to the interfaces are under highest strain, that partly relaxes when moving away from the interface.

The computed increase in C concentration in the narrow tetragonal channels indicates a supersaturation of γ-Fe with C by a factor of 2 or more, in comparison to values obtained from equilibrium phase diagrams. Hence, it is expected that these channels contribute to strengthening by impeding dislocation mobility and affect phase stability by an increase in C diffusivity.

Other activities:

- Invited talk at Linköping University, Sweden
- Best poster award, 3rd International conference on Metals & Hydrogen, Ghent, Belgium

Key publications 2018:

[1] C. H. Liebscher, M. Yao, **P. Dey** et al., Physical Review Materials **2**, 023804 (2018).