Elasto-chemical coupling at coherent interfaces in nano-precipiation strengthened steel revealed by atomic scale correlative microscopy

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A powerful route of designing materials with outstanding mechanical properties is achieved by the dispersion of nanoscale, coherent precipitates in a solid solution matrix phase. Ideally, the precipitate phases themselves exhibit excellent mechanical stability and their lattice parameter mismatch with the surrounding matrix is small. Exactly this lattice mismatch determines the distribution of the precipitates, their stability against coarsening and the interaction with dislocations under an applied stress. Moreover, complex stress states develop around the nano-precipitates that affect the elastic self-interaction of adjoining precipitates and the local chemical equilibrium at the coherent interfaces.

Here, we demonstrate a novel nano-metrological approach correlating aberration-corrected scanning transmission electron microscopy (STEM), atom probe tomography (APT) and density functional theory (DFT) to unravel the coupling of elastic effects at coherent interfaces on the carbon (C) distribution in a nano-precipitation strengthened low-density steel [1]. In this alloy, the face-centered cubic (fcc) iron (Fe) matrix is strengthened by coherent κ-carbide precipitates with a size of 10 to 50 nm [2]. Needle-shaped APT specimen are prepared in such a way that <001> corresponds to the tip axis and are welded on electropolished Mo half-grids for STEM observation. Fig. 1 a shows an overview high angle annular dark-field (HAADF) STEM image and the corresponding 3D-APT reconstruction. Atomic resolution STEM images are obtained in close vicinity of the apex of the tip. A serial acquisition scheme and subsequent non-rigid image registration [3] are employed to reduce the influence of scan noise on the obtained atomic resolution images. This procedure allows to quantitatively determine lattice strains across the coherent interfaces. Moreover, the knowledge of the crystallography of preceding STEM observations was used to calibrate the APT reconstruction to also provide compositional information with highest possible spatial resolution.

It is found that the fcc-Fe matrix is tetragonally strained in nanometer sized matrix channels, as can be seen from quantitative HAADF-STEM images in Fig. 1 b. Especially, the detection of light elements, such as C, remains challenging in the STEM and hence the correlation with APT is employed to explore the effect of coherency strains on composition. The direct correlation of STEM and APT at atomic resolution is illustrated in Fig. 2, illustrating a region containing broad (γ_1) and narrow (γ_2) fcc-Fe matrix channels. An excellent agreement is obtained in determining the location of the interfaces between κ-carbides and fcc-Fe. In APT, no difference in compositional gradients of the broad and narrow matrix channels is found. However, DFT calculations, that are informed by the STEM and APT experiments, predict that the observed tetragonal distortion in the narrow fcc-Fe matrix channels promotes an increase in C solubility. Limitations of the correlative microscopy approach and the atomistic origins of the elasto-chemical coupling will be discussed in detail.

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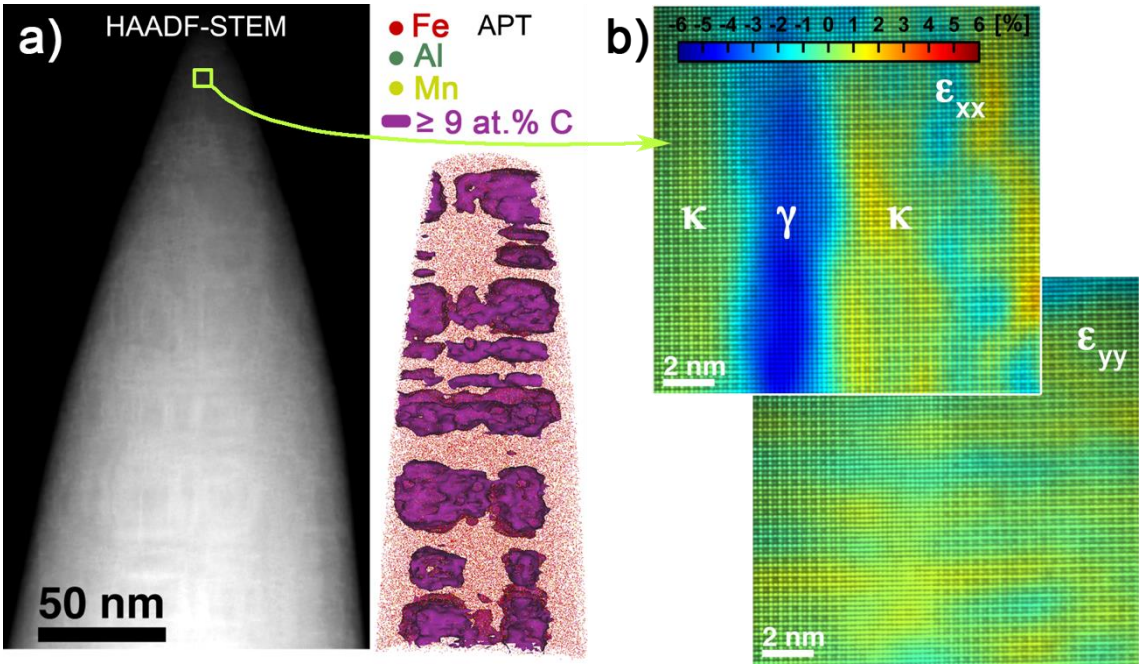

Figure 1: a) HAADF-STEM overview image and corresponding APT reconstruction of the same specimen. b) Atomically resolved HAADF-STEM images and corresponding strain maps determined from the atomic column positions for horizontal (ε_{xx}) and vertical (ε_{yy}) strain components. The region on the specimen for strain determination is indicated by a green square in a). γ indicates a narrow matrix channel and κ the adjacent precipitates.

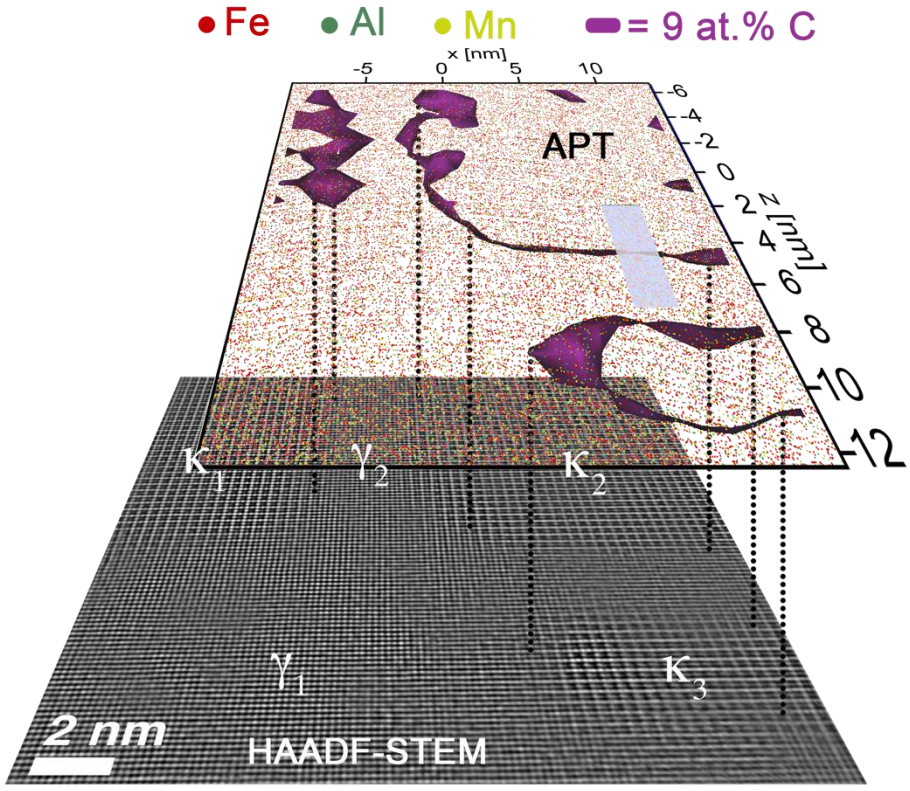

Figure 2: Direct 1:1 correlation of atomic resolution HAADF-STEM and 3D-APT. γ_1 and γ_2 are indicating broad and narrow matrix channels, respectively. κ_1, κ_2 and κ_3 are corresponding three κ-carbide precipitates.