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Multi-Dimensional Machine Learning Aided Analysis of a Nickel-Based Superalloy

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In the wake of improved X-ray detector efficiencies [1] and advanced data processing techniques [2-3] emerges the practicality of multi-dimensional electron microscopy, an analytical approach to materials characterization that combines spatial and spectral information [4]. In this work we combine electron tomography with energy dispersive X-ray (EDX) spectroscopy, a technique some term 4D microscopy, to obtain three-dimensional (3D) chemical information at the nano-scale. Such information is essential to fully understand structure-property relationships in materials. The approach is used to analyze a next-generation nickel-based superalloy, a critically important high strength material used in the aerospace and power industries. Mapping the 3D distribution of the alloying elements, both common and exotic, is essential to better understand the structural origin of its exceptional strength and ultimately aid the design of new superalloys capable of withstanding increased service temperatures.

Here, a 180^0 EDX spectrum image tomographic series is acquired from a focused ion beam-prepared superalloy needle specimen. The large 4D dataset is subsequently analyzed using a machine learning algorithm implemented in HyperSpy [5], called independent component analysis (ICA), to swiftly identify the major spectral components in the tilt series belonging to the individual phases present in the alloy. These components are found to be spatially and chemically representative of the matrix (gamma) and precipitate (gamma’) phases present in the superalloy, enabling their size, distribution and composition to be conveniently and efficiently reconstructed in 3D (Fig. 1). The calculated composition of gamma and gamma’ component spectra are in excellent agreement with atom probe data [6], providing the necessary validation of the machine learning-based analysis approach.

The use of ICA on a tomographic tilt series dataset promises to be a powerful and efficient methodology to perform full 3D chemical analysis on a variety of nano-scale systems [7].

References:

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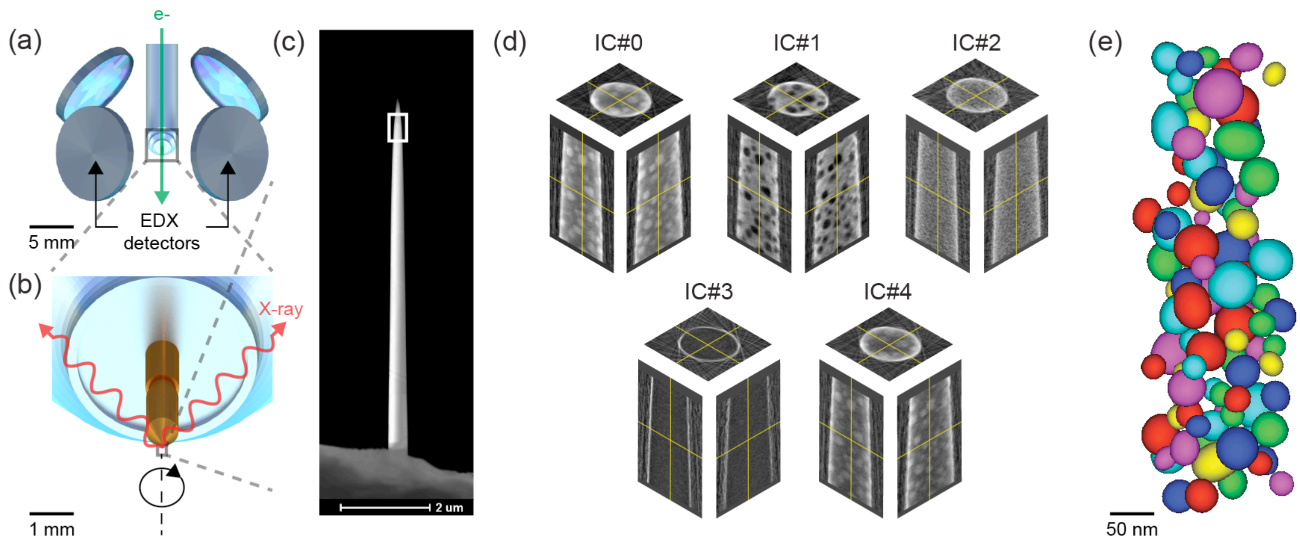

Figure 1. (a) The EDX detector geometry in relation to the on-axis specimen holder. (b) The acquisition of a 180^0 EDX spectrum image tilt series of a needle specimen. (c) The selected region of interest close to the needle tip. (d) The ICA component 3D reconstructions. (e) Segmentation of the gamma' strengthening phase.