doi:10.1017/S1431927622009035
Microsc. Microanal. 28 (Suppl 1), 2022

Role of Nanoscale Coherent Precipitates in Microstructure Evolution of NiTi-based Shape Memory Alloys

Eitan Hershkovitz[1], Yang Yang[1], Michele V. Manuel[1] and Honggyu Kim[1]

[1.] Department of Materials Science Engineering, University of Florida, Gainesville, FL, USA

Shape Memory Alloys (SMAs) are a class of metallic materials that can recover their original shape upon heat treatment after deformation. This unique property has made SMAs a material of interest for a wide array of industrial applications, such as medical devices, actuators, and key structural components for satellites and aerospace vehicles [1]. However, the application of traditional SMAs, *e.g.*, binary NiTi alloys, is largely limited to low service temperature (<100 C°) due to low phase transformation temperatures and structural instability during thermal and mechanical loading. Formation of nanoscale coherent precipitates in the parent matrix of SMAs has been used as an effective means to not only increase phase transformation temperatures, but also enhance the alloy's yield strength. Thus, precipitation-strengthening is becoming increasingly important for the development of high-temperature SMAs. While the strain fields created by nanoscale precipitates are expected to have profound effects on the microstructure evolution and phase transformation behavior, a lack of experimental evidence exists regarding the pattern and extent of strain fields around coherent precipitates and their relationships with the surrounding matrix structure, which poses a challenge in establishing robust alloy design strategy for high temperature applications. Here, we characterize the atomic structure of NiTi-based SMAs at room temperature using aberration-corrected scanning transmission electron microscopy (STEM) to understand how the coherent precipitates impact the microstructure of low-temperature martensite phase. This research serves as a preliminary study for future *in situ* heating experiments to unveil how observed structural properties (*i.e.*, strain field and orientation) of precipitates affect phase transformation behavior in NiTi-based SMAs. These results will be presented at the conference.

We investigate NiTi-based SMAs alloyed with Hf and Al additions using high-angle annular dark-field (HAADF) imaging in STEM. Rigid image registration and two-dimensional Gaussian peak fitting were used to reliably measure atomic column positions, from which lattice parameters can be determined. We develop customized Python scripts to obtain quantitative structural information (*e.g.*, bond distances/angles and strain fields) that goes beyond the detection and classification of crystal structure information.

Figure 1(a) shows a HAADF-STEM image of a NiTiHfAl alloy at the boundary between the matrix and precipitate. The corresponding intensity map shown in Fig. 1(b) is obtained by measuring the atomic column intensity of the nominal Ti sublattice where Hf is mixed with Ti. Figures 1(c-d) visualize the vertical and horizontal bond lengths of the Ti sublattice, respectively. The precipitate is seen near the top of the image as evidenced by its brighter intensity due to the higher concentration of heavy Hf atoms. The dark region, circled in red, at the interface in Figs. 1(a-b) is indicative of a Hf depletion region. We conclude that the viewing axis of the precipitate structure is $[100]_o$, where the subscript refers to the orthorhombic structure, which matches a reported experimental result [2]. In Figs. 1(c-d), we identify a characteristic bond length pattern in the matrix, alternating short (blue) and long (red) bond lengths, indicated by blue and red arrows. A similar characteristic is seen in the bond angle maps shown in Figs 2(a-b), which visualize the bond angle deviation from 180° in Fig. 1(a) by measuring the angle across three collinear atomic columns in the horizontal or vertical directions of the Ti sublattice. These angle maps reveal streaking features in the matrix with systematic ±6° bond angle deviation from 180°. These unique bond length and bond angle patterns in the matrix indicate the matrix phase is closely matched with the twinned martensitic B19 structure (orthorhombic) [3,4]. Here, we demonstrate that quantitative analysis of HAADF-STEM images provides the structure information of both the matrix and precipitate with spatial variation of lattice parameters. Using this quantitative image analysis along with *in situ* heating experiments, we will discuss the dependence of the matrix structure, both high-temperate austenite and low-temperature martensite phases, on coherent precipitate characteristics.

References:
[1] J. Ma *et al*, International Materials Reviews, **55:5**, (2010), p. 257-315. doi:10.1179/095066010X
[2] F. Yang *et al*, Acta Materialia, **61**, (2013), p. 3335-3346. doi: 10.1016/j.actamat.2013.02.023
[3] T. Yu *et al*, Acta Materialia, **208**, (2021), p. 116651. doi:10.1016/j.actamat.2021.116651
[4] J. Chen *et al*, Mater. Res. Express **8**, (2021), p. 106508. doi:10.1088/2043-1691/ac2b57

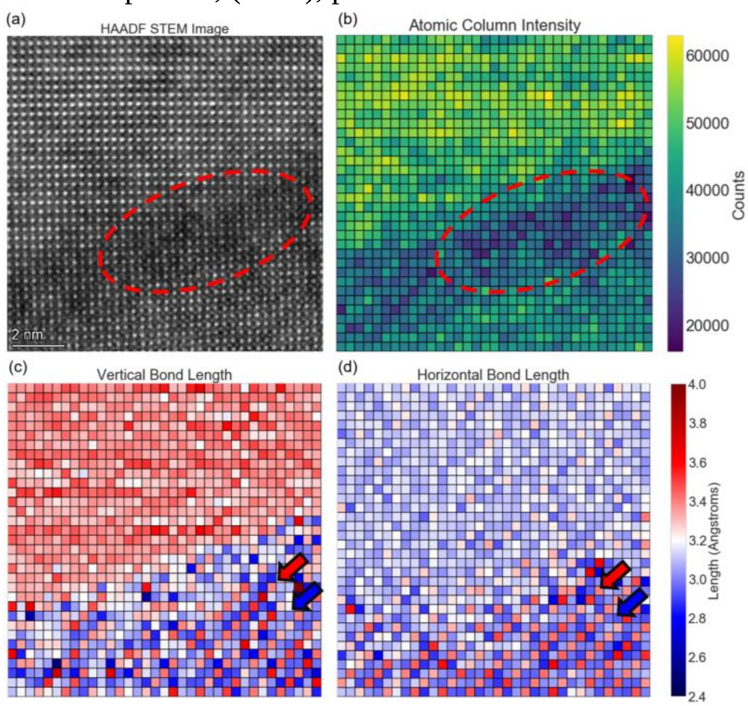

Figure 1. (a) HAADF-STEM image of precipitate matrix interface. (b) Corresponding intensity map with Hf depletion region circled in red. (c) Vertical and (d) horizontal bond length maps measured using the Ti sublattice with arrows showing alternating lengths

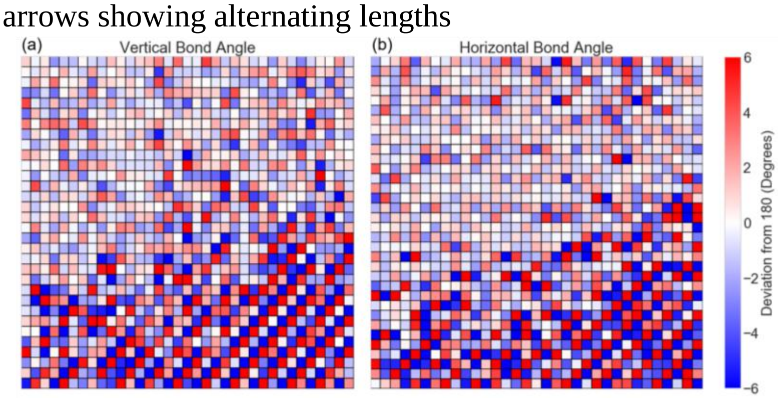

Figure 2. (a) Vertical and (b) horizontal bond angle maps obtained from the Ti sublattice using the image in Fig.1 (a).

https://doi.org/10.1017/S1431927622009035 Published online by Cambridge University Press