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# Coupling Atom Probe Tomography with Aberration-corrected Scanning Transmission Electron Microscopy and First-Principles Computations to Investigate Omega Precipitation in Titanium Alloys

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Perhaps the most studied among all metastable phases in titanium metallurgy is omega phase. It is a submicroscopic precipitate that is supposed to be a transition phase formed during the beta to alpha transformation. These omega precipitates are highly refined (nanometer scale), homogeneously distributed, and can potentially act as heterogeneous nucleation sites for the precipitation of the equilibrium alpha phase. Ever since the discovery of omega phase, researchers have been intrigued by the influence this phase has on the mechanical and superconducting properties of titanium and zirconium alloys.

The present study primarily focuses on omega precipitation within the beta (body-centered cubic or bcc) matrix of simple model binary titanium-molybdenum (Ti-Mo) alloys. Direct atomic scale observation of pre-transition omega-like embryos in quenched alloys, using atom probe tomography coupled with aberration-corrected high-resolution scanning transmission electron microscopy will be presented [1,2]. Atom probe and HAADFHRSTEM observations indicate that the omega transformation is confined with the Mo depleted pockets suggesting a compositionally dependent displacive transformation. Further annealing leads to the coarsening of omega phase and above two techniques are again coupled to study the structural and compositional transitions across the omega/beta interface [3].

Further first-principles computations have been also performed using the Vienna ab initio simulation package (VASP) to determine the minimum energy path for the beta to omega transformation [1] in Ti-Mo alloys with up to 20wt%Mo and the results of these computations will be compared and contrasted with the results from the Atom Probe and HAADF-HRSTEM characterization studies.

References:

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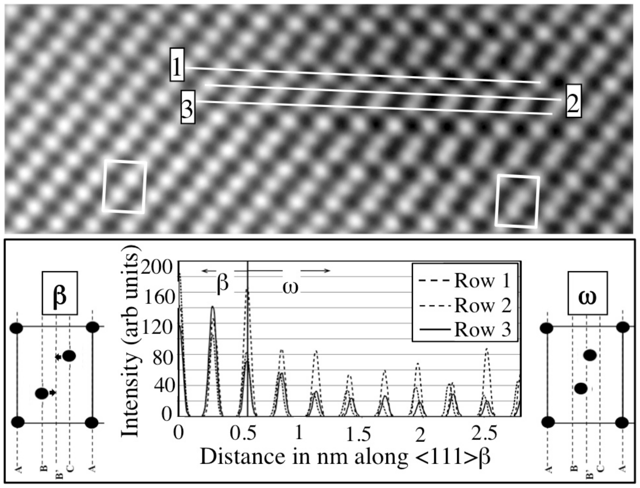

**Figure 1.** Enlarged HAADF-HRSTEM image of rapidly cooled Ti-9 at.% Mo sample showing the undisplaced and partially displaced atomic columns within the beta matrix and omega embryo, respectively. The plot below shows the column intensities along rows 1, 2, and 3 as a function of distance along <111>beta directions. On both sides of the plot, cartoons show the arrangement of atoms as seen from the <110>beta zone axis, along with the beta and partially collapsed omega motifs. [1]

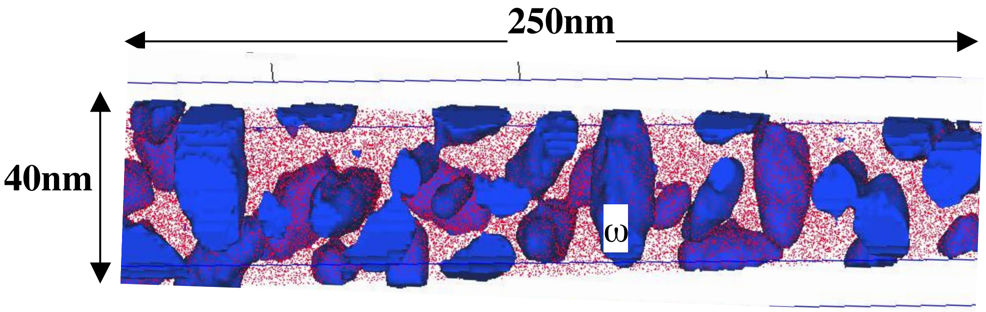

**Figure 2.** Atom probe tomography reconstruction of quenched and annealed Ti-9at%Mo sample showing Ti-rich ellipsoidal omega precipitates of different sizes and orientations [3].