Thermodynamic formation mechanism of nitride nano cluster in iron

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Next-generation automobiles require surface hardening materials for high-torque gearboxes with excellent fatigue and wear resistance. Recent studies have confirmed the presence of nanoclusters in steels, formed by substitutional and interstitial solute elements, which significantly enhance surface hardness [1]. To leverage this mechanism, it is crucial to predict the clustering ability of these elements. We employed first-principles calculations of solute atom distributions to predict microstructures based on alloy composition and heat treatment. The thermodynamic basis of cluster formation was analyzed using free energy data from these calculations.

A two-sublattice model in BCC Fe was used, with N and vacancies in octahedral interstitial sites, and Ti in Fe atomic sites. Various ordered structures were evaluated through first-principles calculations, and effective cluster interactions were derived using the cluster expansion method. Monte Carlo (MC) simulations were then used to study the equilibrium distribution of solute atoms at different temperatures, with N concentration controlled by the chemical potential difference (Δμ) between N and vacancies. Ti content was varied from 1% to 5% in 1% intervals. Data on solute distribution were collected by changing the temperature from 400 to 1000 K in 50 K steps.

Figure 1 shows results for Fe-1at.%Ti at 500 K. Figure 1(a) depicts the equilibrium N concentration as a function of Δμ, with N concentration increasing as Δμ increases. Figures 1(b) and 1(c) show equilibrium atom distributions for Δμ = 200 meV and Δμ = 300 meV, respectively. N atoms are gray, and Ti atoms are light blue. Figure 1(b) replicates the plate-like clusters observed experimentally, while Figure 1(c) shows a uniform Ti distribution. Higher N concentration leads to smaller Ti clusters surrounded by N, inhibiting plate-like cluster formation. In the presentation, similar calculations are used to discuss the short-range ordering in high-entropy alloys (HEAs).

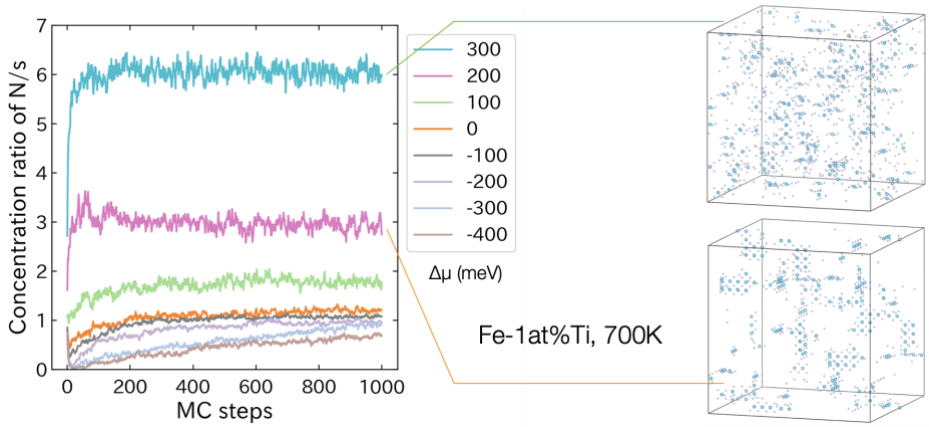

Fig.1: Results of calculations for the Fe-1at.%Ti alloy performed at T = 500 K.

[1] G. Miyamoto, Y. Tomio, H. Aota, K. Oh-ishi, K. Hono, and T. Furuhara, et al., Mater. Sci. Tech., 27(2011)