# Density functional theory study of ω-phase in steel with varied alloying elements

S. Assa Aravindh[1], Sakari Pallaspuro[1], Wei Cao[1], Mahesh Somani[1], Matti Alatalo[1], Marko Huttula[1], and Jukka Komi[1]

[1]University of Oulu

May 5, 2020

**Abstract**

The presence of long abandoned, hexagonal omega (ω) phase in steel samples is recently gaining momentum on account of accurate transmission electron microscopy (TEM) measurements. The formation and stabilization of this metastable phase down to room temperature is attributed to the combined effect of factors such as accelerated cooling, special atomic constraints at twin boundaries, and the enrichment of solute elements such as Al, Mn, Si, C, and Cr in the nanometer sized regimes. Here, we present a density functional theory (DFT) study of the effect of the above alloying elements in ω-Fe and confirm the predictions using high resolution TEM observations of the structure of an experimental steel at high magnifications. It is found that the FM and ++- spin states are the most stable for a primitive cell of ω-Fe. The density of states calculations show that the d band occupancy of ω-Fe is changing in presence of the alloying elements, and this in turn will affect the cohesive energy. Further, the dynamical stability analysis from phonon band structure reveals that only ω-Fe with substitutional C exhibits thermodynamic stability. This is in line with experimental indications that the stabilization of ω-phase in ferritic/martensitic steels occurs due to the presence of special symmetry constraints at grain boundaries

**Hosted file**

`omega-4-dec.doc` available at https://authorea.com/users/287637/articles/412472-density-functional-theory-study-of-%CF%89-phase-in-steel-with-varied-alloying-elements