

First-principles investigation of alloying element effects on mechanical properties and corrosion susceptibility of advanced high-strength steels

Yan Cheng^{1,2}, Xian Zhang^{1,2}, Lin Cheng^{1,2}, Jing Liu^{1,2}, Kaiming Wu^{1,2}

¹*Department of Applied Physics, College of Science, Wuhan University of Science and Technology, Wuhan 430081, P.R. China*

²*Collaborative Innovation Center for Advanced Steels, Wuhan University of Science and Technology, Wuhan 430081, P. R. China*

chengyan0006@wust.edu.cn

Abstract In the present study, first-principles calculations based on density functional theory (DFT) were performed using the Vienna Ab-initio Simulation Package (VASP) to investigate the effects of alloying elements on the mechanical properties and corrosion susceptibility of Advanced High-Strength Steels (AHSS). The impact of alloying elements on the mechanical properties of α -Fe and γ -Fe was explored by analyzing the differences in elastic constants before and after doping various alloying elements into the iron matrix (Fig.1). Furthermore, the influence of alloying elements on the adsorption behavior of Cl atoms on α -Fe and γ -Fe was examined by comparing the differences in the adsorption energy of Cl atoms before and after doping. (Fig.2).

The results showed that the addition of Mo, Mn, Si, and Ni influenced the mechanical properties of both α -Fe and γ -Fe, and Mo showed the most significant impact on matrix strength. The doping of Si, Ni, and Mn affected the work function and stability of the iron matrices, while Al and Mo influenced the surface energy values. The adsorption energy calculations of Cl atoms revealed different adsorption trends for α -Fe and γ -Fe, with Mn enhancing the adsorption of Cl atoms in both structures. Bader charge analysis indicated complex charge exchange behavior between atoms, influenced by differences in atomic electronegativity and local structure.

The mechanical properties and corrosion resistance influenced by adding alloying elements provide strategies for optimizing AHSS composition and microstructure. The trends in work function, surface energy, and Cl adsorption energy variations with different alloying elements can guide the selection of alloying combinations to enhance AHSS performance in various applications, particularly in corrosive environments. However, Bader charge analysis reveals complex interactions between the alloying

elements and the iron matrix. This highlights the necessity of carefully considering the collaborative effects arising from the interplay of multiple factors.

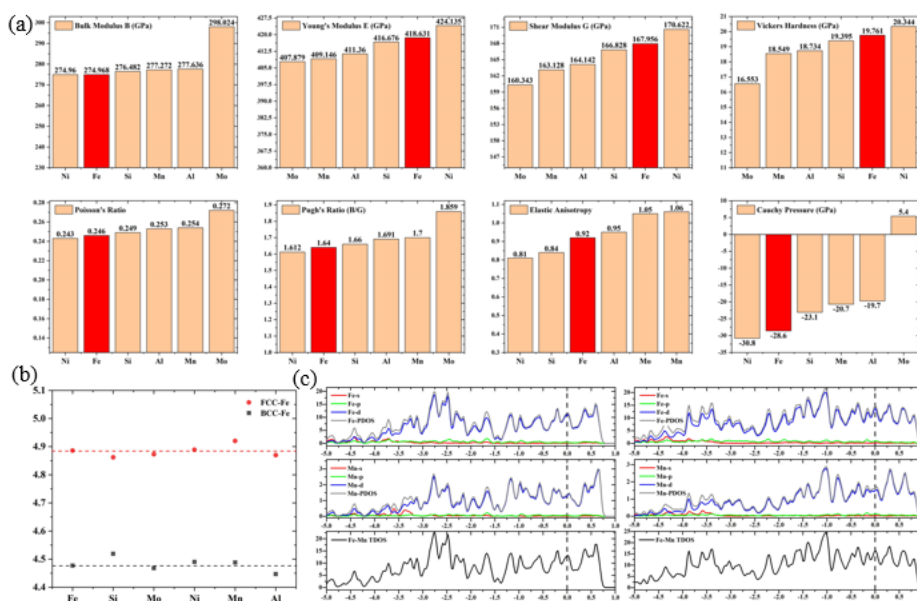


Fig. 1 Comparison of the influences of alloying elements on the steel matrix: (a) Mechanical properties, (b) Work function, (c) Density of states

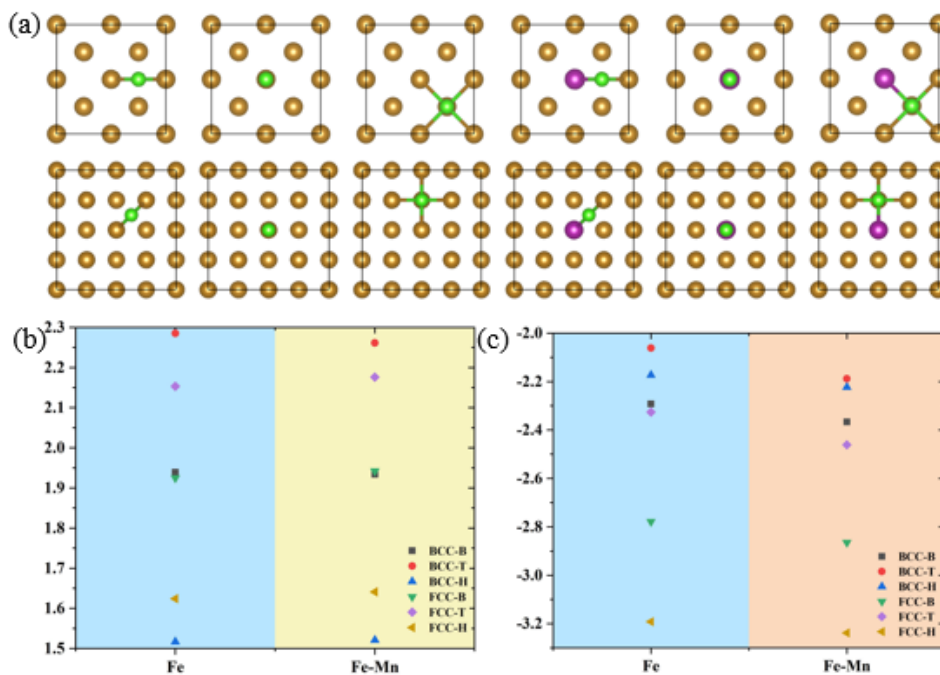


Fig. 2 Comparing the influences of alloy elements on adsorption behavior: (a) Computational models used for calculating the adsorption behavior of Cl atoms, (b) Equilibrium adsorption distance, (c) Adsorption energy

Keywords

First-principles calculation, Mechanical properties, Corrosion resistance, Advanced high-strength steels

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