

Design of High-Strength, High-Conductivity Copper Alloys through Controlling the Precipitation Behavior based on First-Principles Calculations

We investigated precipitation control in Cu-Ti alloys using first-principles calculations to design high-strength, high-conductivity copper alloys. DFT analysis of 22 elements revealed that P and Cr can enhance the cohesive energy of α -Cu₄Ti, reduce its precipitation activation energy, and refine its precipitate size, thereby promoting α -Cu₄Ti precipitation. These insights provide guidance for tailoring precipitation behavior in the development of advanced Cu-Ti alloys.

Cu-Ti alloys can reach tensile strengths above 1 GPa, which makes them promising alternatives to Cu-Be alloys [1]. Aging causes spinodal decomposition, forming metastable α -Cu₄Ti (I4/m) as the strengthening phase, later transforming into β -Cu₄Ti (Pmmn) [2,3]. Due to slow precipitation, optimizing strength and conductivity is difficult. Precipitation behavior depends on cohesive and interfacial energies of α -Cu₄Ti with the Cu matrix. Previous DFT work on 3d transition metals [4] examined these separately but not their combined effect.

Here, we calculate these energies for α -Cu₄Ti doped with 22 alloying elements (Li, Mg, Al, Si, P, Sc, V, Cr, Mn, Fe, Co, Ni, Zn, Ga, Ge, Y, Zr, Nb, Mo, In, Sn, Hf), derive precipitation activation energy and critical length, and identify elements that promote finer precipitation. First-principles DFT with PAW and PBE in VASP was used. Supercells for bulk α -Cu₄Ti and two major interfaces with Cu were fully relaxed. Alloying elements were substituted into Cu or Ti sites at 6.25 at.%.

Twelve elements (P, Cr, Mn, Fe, Co, Ni, Mo, Li, Sc, Y, Zr, and Hf) increased cohesive energy (E_{coh}), stabilizing α -Cu₄Ti. Mn was effective at both sites. Interfacial energies (E_{int}) were computed for Cu (001) // α -Cu₄Ti (001) and Cu (310) // α -Cu₄Ti (100). Among twelve dopants enhancing E_{coh} , only P and Cr lowered E_{int} at Cu (001) // α -Cu₄Ti (001) interface by relieving lattice mismatch, but increased it at Cu (310) // α -Cu₄Ti (100).

Total energy curves combining E_{coh} and E_{int} were analyzed against precipitate size. Figure 1, for Cr-doped α -Cu₄Ti, shows reduced precipitation activation energy (E_a) and critical length (L_c) compared with undoped alloy. P and Cr lowered E_a by 21%

and 37% and reduced L_c by 11% and 26%, forming smaller, more uniform precipitates. Mn, Co, and Ni increased E_a but reduced L_c , indicating some refinement effect.

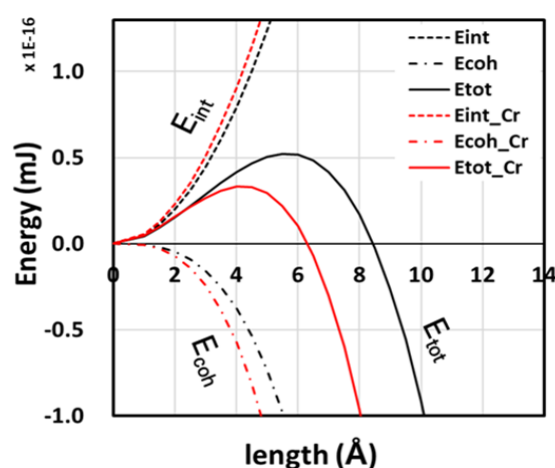


Fig. 1 The cohesive, interfacial and total energies for α -(Cu_{0.94}Cr_{0.06})₄Ti as a function of the length of precipitate. The black line represents the energies of the undoped one.

In conclusion, P and Cr are the most effective additives, stabilizing α -Cu₄Ti and enhancing precipitation, offering a pathway to high-performance Cu-Ti alloys with tailored microstructures.

References

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