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The effect of V content on the magnetic and mechanical properties of B2 FeCo alloy: a DFT approach

FeCo alloy plays an important role in soft magnetic materials with a wide range of technological applications due to their high saturation magnetization and Curie temperature. However, this binary alloy displays poor ductility at room temperature. The ductility of this alloy can be improved by the ternary addition of V. In this study, the HPC application code VASP was used and a supercell was used to generate B2 Fe50Co50-X-VX structures and different properties were evaluated at different atomic percentage compositions to determine their ductility at room temperature. The structures were fully optimized and provided reliable equilibrium ground-state properties for both binary and ternary systems, with the lattice parameters in better agreement with experimental data. The stability of the Fe50Co50-X-VX was evaluated from the heats of formation, elastic properties, magnetic properties, and phonon dispersion curves. It was found that all structures are thermodynamically stable due to negative heats of formation. In addition, the Pugh ratio (B/G) and Poisson's ratio confirm that alloying with V effectively improved the ductility. It was also found that Fe50Co50-XVX showed positive shear modulus, condition of stability for the entire concentration range in agreement with phonon dispersion curves. This implies that the ternary addition of V on the FeCo system resulted in enhanced magnetic properties, suggesting that Fe50Co50-X-VX alloys can be used in the future development of magnets

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