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Toward high-performance iron based alloys: Ab initio study

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Car industry has required light-weight steels, but still with strong mechanical strength. To meet this requirement, a variety of researches on Fe-Al alloys have been performed. As Al is being added in a disordered manner, alloys become more ductile and show higher yield stress. At a certain concentration of Al, however, the Fe-Al alloy system falls in a second phase whose mechanical strength is worsened. To understand the microscopic role of Al, we investigate the stability and the elastic properties of various Fe-Al alloys using *ab initio* density functional theory. At agiven Al concentration ,the equilibrium geometry is obtained among several disordered Fe-Al alloy structures by performing the geometry relaxation. The formation energies and elastic properties such as bulk moduli of the equilibrium structures are also computed as a function of Al concentration. We also investigate the effects of different elements such as Si and Mn. Fe-Si alloy systems exhibit unusual mechanical behaviors requiring further investigation to understand their physical origin. Especially, the microscopic role of Mn is investigated to find its physical origin of preventing the Fe-Al alloy system from forming an unfavorable second phase. The effect of manganese on mechanical properties of Fe-based alloys is also explored.