On the *ab initio* prediction of the mechanical properties of alloys: The case of Ni/Mn-doped ferromagnetic Fe

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First-principles alloy theory, formulated within the exact muffin-tin orbitals method in combination with the coherent-potential approximation, is used to study the mechanical properties of ferromagnetic body-centered cubic (bcc) $Fe_{1-x}M_x$ alloys (M = Mn or Ni, $0 \leq x \leq 0.1$). We consider several physical parameters accessible from *ab initio* calculations and their combinations in various phenomenological models to compare the effect of Mn and Ni on the properties of Fe. Alloying is found to slightly alter the lattice parameters and produce noticeable influence on elastic moduli. Both Mn and Ni decrease the surface energy and the unstable stacking fault energy associated with the $\{110\}$ surface facet and the $\{110\}\langle 111\rangle$ slip system, respectively. Nickel is found to produce larger effect on the planar fault energies than Mn. The semi-empirical ductility criteria by Rice and Pugh consistently predict that Ni enhances the ductility of Fe but give contradictory results in the case of Mn doping. The origin of the discrepancy between the two criteria is discussed and an alternative measure of the ductile-brittle behavior based on the theoretical cleavage strength and single-crystal shear modulus $G\{110\}\langle 111\rangle$ is proposed.

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