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Alloying Contributions to Twinnability in Nickel: Testing the Rule of Thumb DONALD SIEGEL, US Naval Research Laboratory — It is well-known that the addition of small quantities of solute atoms can dramatically alter the mechanical properties of an unalloyed metal. An example is the change in a metal's tendency to twin after solute incorporation. The rule of thumb describing a solute's effect on twinning is based on changes to the intrinsic stacking fault energy (SFE) of the unalloyed phase: If a solute lowers the SFE, then the twinnability of the alloy should be greater than that of the pure phase. In FCC metals, it is furthermore thought that alloying will lower the SFE if the first intermetallic phase in the binary phase diagram is HCP. By combining *ab initio* simulations with an elasticity theory expression for twinnibility [1], I examine whether the conventional wisdom regarding alloying and twinnability are correct. Using Nickel as a test case, it is first shown that the theoretical twinnability of pure Ni falls within the expected experimental range [1]. I then evaluate the generalized stacking fault surface for Ni with Nb, Mn, and W additions, and compare their twinnability with the rule-of-thumb predictions.
[1] Bernstein and Tadmor, Phys Rev B 69, 094116 (2004)

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