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Phase-Stabilizers in Titanium Alloys BENGT TEGNER, LING-GANG ZHU, GRAEME ACKLAND, SUPA, School of Physics and Astronomy, The University of Edinburgh — Titanium alloys exhibit three distinct crystal structures: alpha, beta and omega. For various applications alloying elements can be used to stabilize the desired phase. While alloy designers have well established rules of thumb, rigorous theory for non-equilibrium single-phase crystal stability is less well established. Here we tackle this problem using electronic structure calculations. We use two different methods based on density functional theory with pseudopotentials and plane waves, with either explicit atoms or the virtual crystal approximation (VCA). The former is highly reliable, while the latter makes a number of drastic assumptions that typically lead to poor results. Surprisingly, the agreement between the methods is good, showing that the approximations in the VCA are not important in determining the phase stability and elastic properties. This allows us to generalize, showing that the single-phase stability can be related linearly to the number of d-electrons, independent of the actual alloying elements or details of their atomistic-level arrangement. This leads to a quantitative measure of beta-stabilization for each alloying transition metal.

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