Abstract Submitted
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Stability in bcc transition metals: Madelung and band-energy effects due to alloying[1] ALEX LANDA, PER SODERLIND, Lawrence Livermore National Laboratory, Livermore, USA, ANDREI RUBAN, OLEG PEIL, LEVENTE VITOS, Royal Institute of Technology, Stockholm, Sweden — The phase stability of Group VB (V, Nb, and Ta) transition metals is explored by first-principles electronic-structure calculations. Alloying with a small amount of a neighboring metal can either stabilize or destabilize the body-centered-cubic phase relative to low-symmetry rhombohedral phases. We show that band-structure effects determine phase stability when a particular Group VB metal is alloyed with its nearest neighbors within the same d-transition series. In this case, the neighbor with less (to the left) and more (to the right) d electrons, destabilize and stabilize bcc, respectively. When alloying with neighbors of higher d-transition series, electrostatic Madelung energy dominates and stabilizes the body-centered-cubic phase. This surprising prediction invalidates current understanding of simple d-electron bonding that dictates high-symmetry cubic and hexagonal phases.

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