

Abstract Submitted
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High-throughput formalism and calculation of Ag, Au, Cd, Co, Cr, Ir, W, and Zn solubility in Ti from first-principles¹ ROMAN CHEPULSKYY, STEFANO CURTAROLO, Duke University — Based on statistical-thermodynamic theory of a dilute lattice gas, we developed an approach for calculation of atomic solubility in alloys. The advantage of the approach consists in taking into account all known alloy ground states rather than just pure species. It is shown that the low-solubility obey the simple Arrhenius-type dependence on temperature determined by “low-solubility formation energy.” Such quantity is defined as the derivative of the compound formation energy, determined with respect to surrounding ground states, versus composition. “Low-solubility formation energy” coincides with the usual “true” defect formation energy only in the case of a phase-separating alloy having no intermediate ground states and vacancies. We present a high-throughput formalism where the “low- solubility formation energy” can be directly obtained through first-principles calculations. The developed approach is applied to solubility of transition metals in titanium. The obtained values and tendencies are in good qualitative correspondence with experiments.

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