Theoretical Approach of Phase Selection in Refractory Metals and Alloys

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First-principles total energy calculations are used to examine the phase stability of the Frank-Kasper (FK) structures. The sequence of FK phases observed as a function of composition in many transition metal binary systems is shown to have a band-filling origin. We show that the alloying effects can be treated using a first-principles statistical thermodynamics approach and first results are given for Re-Ta and Re-W sigma alloys.