Structural complexity in binary bcc ground states: The case of bcc Mo-Ta

Volker Blum and Alex Zunger
National Renewable Energy Laboratory, Golden, Colorado 80401, USA
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alloy system. In the present work, we apply a three-level, iterative construction scheme:

(i) For a given number n_p of pairs and a set of nonpair interactions J_{MB}, one first obtains an optimum interaction set J_f by minimizing[8,20]

$$s_{\mathrm{MBCE}} = \sum_{\sigma} w_{\sigma} \left| \tilde{H}_{\mathrm{LDA}}(\boldsymbol{\sigma}) - \tilde{H}_{\mathrm{CE}}(\boldsymbol{\sigma}) \right|^2 + \frac{t}{\Lambda} \sum_{p}^{n_p} R_p D_p J_p^2 . \quad (3)$$

Here, the usual least-squares sum is amended by an additional constraint per pair. This allows for an unlimited number of pair interactions, and avoids an unphysical cutoff dictated by the finite number of input structures. The proper spatial decay of J_p with pair distance R_p is enforced by weight factors R_p, with t a Lagrangian multiplier and $\Lambda = (\sum_{p}^{n_p} \sqrt{R_p/D_p})^2$ a normalization factor.

(ii

Carlo simulations, cell sizes $20\times20\times20$ or larger, 2000 or 4000 flips per site) based on the converged MBCE.

reciprocal space for 79% Mo and 63% Mo solid solutions.[32] This is confirmed by simulations based on our converged MBCE.

The ground-state structures of regions 3 and 4 are unsuspected in that they cannot exist within a few-interaction ground-state enumeration scheme:[12,13]

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