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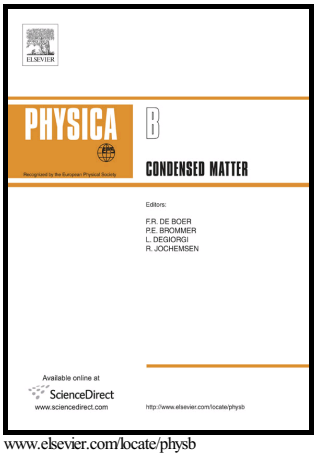

www.elsevier.com/locate/physb

PII: S0921-4526(17)30217-X
DOI: http://dx.doi.org/10.1016/j.physb.2017.04.032
Reference: PHYSB309923

To appear in: *Physica B: Physics of Condensed Matter*

Received date: 10 February 2017
Revised date: 24 April 2017
Accepted date: 29 April 2017

Cite this article as: G. Bonny, N. Castin, M.I. Pascuet and Y. Çelik, Exact mean field concept to compute defect energetics in random alloys on rigid lattices *Physica B: Physics of Condensed Matter* http://dx.doi.org/10.1016/j.physb.2017.04.032

Exact mean field concept to compute defect energetics in random alloys on rigid lattices

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Abstract

In modern materials science modeling, the evolution of the energetics of random alloys with composition are desirable input parameters for several meso-scale and continuum scale models. When using atomistic methods to parameterize the above mentioned concentration dependent function, a mean field theory can significantly reduce the computational burden associated to obtaining the desired statistics in a random alloy. In this work, a mean field concept is developed to obtain the energetics of point-defect clusters in perfect random alloys. It is demonstrated that for a rigid lattice the concept is mathematically exact. In addition to the accuracy of the presented method, it is also computationally efficient as a small box can be used and perfect statistics are obtained in a single run. The method is illustrated by computing the formation and binding energy of solute and vacancy pairs in FeCr and FeW binaries. In addition, the dissociation energy of small vacancy clusters was computed in FeCr and FeCr-2%W alloys, which are considered model alloys for Eurofer steels. As a result, it was concluded that the dissociation energy is not expected to vary by more than 0.1 eV in the 0-10% Cr and 0-2% W composition range. The present mean field concept can be directly applied to parameterize meso-scale models, such as cluster dynamics and object kinetic Monte Carlo models.

Keywords: atomistic modelling; random alloys; rigid lattice

1. Introduction

In modern materials science modeling, the evolution of the energetics of random alloys with composition are desirable input parameters for several meso-scale and continuum scale models. On the continuum scale, several thermodynamic packages (MatCalc, ThermoCalc, FactSage…) [1-3] hinge on an accurate description of the free energy of random solid solution, even outside their experimental stability range. On the meso-scale, cluster dynamics models [4] and object kinetic Monte Carlo methods [5-7] hinge on an accurate description of