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Development of bond-order potentials for bridging the electronic to microstructural modelling hierarchies in materials science

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A multi-scale modelling framework suitable for guiding the design of advanced alloys and steels must take into account defects, impurities and complex phases within its remit. As electronic structure calculations based on density functional theory are computationally expensive, there is a need for more simple yet robust interatomic potentials that are capable of describing defects and complex phases. In my talk I will show how interatomic potentials may be derived by systematically coarse-graining the electronic structure into effective interatomic interactions. The resulting analytic bond-order potential (BOP) may be regarded as a systematic extension of the second-moment Finnis-Sinclair potential to include higher moments. The analytic BOP depends explicitly on the valence of the transition metal element and predicts the structural trend from hcp to bcc to hcp to fcc that is observed across the non-magnetic 4d and 5d transition metal series. The potential also describes the different ferromagnetic moments of the alpha (bcc), gamma (fcc) and epsilon (hcp) phase of the 3d transition metal iron, the difference between the ferromagnetic and anti-ferromagnetic states as well as non-collinear spin-configurations. In addition, this new potential includes a correct description of alloy bonding within its remit. This analytic BOP may then be used in large scale atomistic simulations in order to derive the format as well as the parameterizations of microstructural models and in this ways for bridging to the microstructural length scale.

R. Drautz and D.G. Pettifor, Phys. Rev. B 74, 174117 (2006).

Mardi 18 Septembre 2007 à 10h30

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