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Tight-binding study of impurity problems in BCC transition metals DANIEL FINKENSTADT, Naval Research Laboratory, DIMITRIOS PAPACONSTANTOPOULOS, George Mason University, MIKE MEHL, Naval Research Laboratory — Tight-binding provides a useful theoretical framework for studying defects and impurity problems, that would otherwise be very computationally demanding using density-functional and all-electron first-principles methods. Here we extend our tight-binding formalism, the NRL tight-binding method, to include alloy cases, specifically for BCC transition metals and their impurity formation energies. We have used a virtual-crystal approximation (VCA) of the impurity, onsite and hopping TB parameters, and we find that in many cases the VCA gives reasonable results for lattice and elastic constants, as well as for predicting correct ground-state structures. The VCA is then applied to calculate substitutional impurity defect energies and also interstitial defect energies, that we have examined previously with in tight-binding [PRB, in press, 2006].

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