

Analytic bond-order potentials for modeling the growth of semiconductor films

D.G. Pettifor¹, R. Drautz¹, D. Nguyen-Manh², D.A. Murdick³, X.W. Zhou³ and H.N.G. Wadley³

¹Department of Materials, University of Oxford; ²UKAEA Fusion, Culham Science Centre;

³Department of Materials Science and Engineering, University of Virginia.

ABSTRACT

Robust interatomic potentials for simulating the growth of semiconductor films should be able to describe bond breaking and remaking naturally within their remit. In this paper we outline the derivation of such potentials, the so-called bond-order potentials (BOPs), by performing a systematic coarse graining from the electronic to atomistic modeling hierarchies. First the density functional theory (DFT) electronic structure and binding energy is simplified by introducing the tight-binding (TB) bond model whose parameters are determined directly from the DFT results. Second, this TB electronic structure is coarse grained through atom-centered moments and bond-centered interference paths, thereby predicting the analytic form of the interatomic BOP. We show that these interatomic potentials predict structural energy differences in quantitative agreement with k-space TB calculations and reproduce the experimental structural trends across the sp-valent elements. We discuss the current development of these potentials for simulating the growth of Si and GaAs films.