



Invited Talk, Monday, May 6, 11:40 a.m. - 12:20, ICAMS² session: **M1**

Bond-order potentials for BCC transition metals with attraction determined by bond integrals deduced from DFT and repulsion from the overlap of p electrons of closed-shell atoms of argon

Yi-Shen Lin¹, Matous Mrovec^{2,3}, and Vaclav Vitek¹

¹*Department of Materials Science and Engineering, University of Pennsylvania, 3231 Walnut Street, Philadelphia, PA 19104, USA*

²*Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstraße 11, D-79108 Freiburg, Germany*

³*Institute of Applied Materials – Reliability of Components and Systems IAM-ZBS, Karlsruhe Institute for Technology KIT, Kaiserstraße 12, D-76131 Karlsruhe, Germany*

While the most rigorous atomistic calculations are at present based on the density functional theory, this approach is very limited when studying extended defects owing to a small number of atoms that can be included and application of periodic boundary conditions. Consequently, the problem needs to be coarse grained such that atoms are assumed to interact via interatomic potentials. For transition metals in which the cohesion is controlled by the partially filled d-band, one of the most attractive schemes is the bond order potentials (BOPs) based on the tight-binding model that captures the essential aspects of mixed covalent and nearly-free electron bonding [1-3]. Very importantly, this scheme can be employed purely in the real space.

Within any tight-binding scheme the energy of the system studied consists of two separate parts, attractive and repulsive that are not differentiated in DFT calculations. The attractive part is determined rigorously quantum mechanically using well-defined approximations such as two-centre bond-integrals and limitation to a chosen number of moments of the density of states when deriving BOPs. On the other hand, the repulsive part is an empirically fitted dependence on the relative positions of particles with varying physical justification. However, in atomistic studies that involve relaxations of atomic positions the two parts of the energy are equally important. In the earlier development the bond integrals were obtained by employing DFT calculations for the whole s, p and d basis orthogonalised before limiting to the $dd\sigma$, $dd\pi$ and $dd\delta$ integrals needed when considering only d-bonding. These bond integrals had to be screened to remove the effect of s and p orbitals [4]. The repulsive part that needs to be environment dependent to be able to reproduce elastic constants was described by an empirically fitted Yukawa form [5].

In this paper we present BOPs for a number of BCC transition metals (Mo, Ta, W, Nb, V, and Fe) that are based on two new advances. First, the bond integrals have been developed via simultaneous optimisation and projection of atomic-like orbitals on self-consistent DFT wave functions and do not require screening since they are limited to d-types before orthogonalisation [6]. Secondly, the environment dependent repulsion, while still empirical, is based on the quantum mechanical investigation of the overlap repulsion of p electrons in closed-shell atoms of argon [7]. Since the physical origin of the repulsion via the overlap of p electrons is the same in transition metals it is our conjecture that the functional form of this repulsion will be the same. For the developed BOPs we investigate their transferability to defective structures by comparing DFT and BOP calculations of the stability of alternate structures, transformation paths, vacancies, phonons, γ -surfaces and cores and glide of 1/2 [111] screw dislocations that govern the mechanical behaviour of BCC metals.

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