



ICAMS special lecture

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Wednesday, July 9, 10:30 a.m. ICAMS conference room IC 02/574/508

Importance of screening of bond integrals in BOPs for transition metals

In this talk we shall discuss two aspects that need to be carefully considered when studying the core of $\frac{1}{2}\langle 111 \rangle$ screw dislocations in BCC transition metals and their response to externally applied stresses. The first is the importance of the core displacements perpendicular to the Burgers vector. This part is general and applies equally to all potentials and elucidates the difference between atomic interactions that are purely central force and those including directional bonding. The second aspect concerns specifically BOPs. Here we compare the results of screw dislocation studies made with BOPs based on bond integrals with and without screening of s electrons positioned at neighbouring atoms of a given dd bond. This demonstrates that while the core displacements parallel to the Burgers vector are virtually the same in both cases, the core displacements perpendicular to the Burgers vector are entirely different. This difference then leads to a very different response of the dislocation to stresses other than pure shear in the direction of the Burgers vector that appears to be unphysical in the unscreened case.