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Reconstruction of atomistic models of dislocation networks, based on lattice distortion tensor fields algebra

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ABSTRACT

Dislocation networks in monocrystalline heterostructures compose metastable configurations of crystal lattice. Mostly the atomistic models of misfit dislocation networks are obtained as a result of plastic deformation simulations. Such approach does not give possibility to reconstruct of an arbitrary chosen atomistic model of dislocations with the fixed geometry of the dislocation network assumed. Contrary to that, atomistic models of single dislocation cores as well of a few dislocation cores are preprocessed by the use the Love equations for discontinuous displacement field from single dislocation. This method is generally used in ab-initio calculations. In this presentation we show why the more complex dislocation networks composed for example of several dislocation lines stored in a periodic cell cannot be obtained in this way as of yet. The reason does not lie in the elastic nonlinearity nor in the finite deformation approach required in preprocessing but does in the missing of the correct analytic solutions for dislocation lines considered in atomistic terms. For example, in the Hirth and Lothe textbook, over 90% all analytic solutions are based on the assumption that the whole Burgers vector of dislocation is stored only in the elastic strain field incompatibility.

By comparison, the correct analytic solution presented by Love is composed of the singularity of lattice distortion field stored both in the strain field and rotation field. Integration of the mentioned distortion field over Burgers circuit proves that in the Love solution only the half of the Burgers vector is stored in the strain field but the remaining half is stored in the rotation tensor field incompatibility stored in dislocation core. Thus, in order to use analytic solutions for reconstruction of advanced atomistic models of dislocation networks, the analytic solutions for rotation tensor fields must be rescued by solving once more the analytic problem for dislocations with the use of the rotation field singularity. We show also to which (incorrect) atomistic models lead the use of analytic solutions for dislocations based on strain field only.

The method presented here gives possibility for the vector editing of dislocations and preprocessing of assumed geometric configuration of dislocations. This method is developed by the authors with the use of the *Visual Editor of Crystal Defects* (VECD). Such obtained configurations of dislocation networks can be used next as input data for the ab-initio and/or molecular dynamics programs in order to compare each other the energy of different dislocation networks.

Keywords: Ab-initio, atomistic modeling, tensor fields, dislocation fields algebra, lattice distortions, visualization methods