Title Preprocessing of atomistic models of dislocations based on finite deformation approach

Description Dislocations and their long-range elastic deformation field play an important role in prediction of various physical properties of crystal structures. Among others, this concerns semiconductor epitaxial layers where dislocations compose nonradiative recombination centers. Also, an emission spectrum which is a very important parameter for optoelectronic device depends on the formation energy related to the atomic configuration of dislocation cores. Despite the very promising electronic properties of many semiconductors the defect formations which arise during the growth process compose a technological barrier for application of such obtained structures in optoelectronic devices. Experimental measurement in that domain, mainly by the X-ray methods and transmission electron microscopy are very tricky, therefore atomistic simulations have become a common method for investigating dislocation phenomena [1]. Despite real crystals demonstrate an anisotropic behavior, currently one of most popular analytic approaches to the preprocessing of atomistic models of misfit dislocation sets fixed in the given position of crystal lattice is based on the use of Love's equations and its various modifications [2]. It is worth mentioning that many of known analytic solutions for misfit dislocations are based on the use of a strain tensor field. In such a case the Burgers vector is determined directly as the integral of strain field over the Burgers contour. By neglecting (often unknown) rotation tensor field such models overestimate the elastic energy of dislocation cores a few times. In this presentation it is shown how far the proper coupling of the misfit rotation and misfit strain tensor fields in the preprocessing decrease the energy stored in such reconstructed dislocation cores. References 1. Dluzewski P., Domagala J.Z., Kret S., Jarosz D., Krysko M., Teisseyre H., Phase-transition critical thickness of rocksalt $Mg_xZn_{1-x}O$ layers, Journal of Chemical Physics 154, 154701 (2021). 2. Cholewinski J., Mazdziarz M., Jurczak G., Dluzewski P., Dislocation core reconstruction based on finite deformation approach and its application to 4H-SiC crystal, Journal for Multiscale Computational Engineering 12, 411–421 (2014).

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