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A FINITE ELEMENT APPROACH FOR THE ANALYSIS OF VARIABLE CORE DISLOCATIONS

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A finite element description of variable core edge dislocations in the context of linear elasticity is presented in this work. The approach is based on a thermal analogue and the integral representation of dislocations through stresses [1]. The stress fields of a single edge dislocation in classical isotropic elasticity break down at distances near the dislocation core and lead to r^{-1} singularities, which in turn result in logarithmic singularities for the total strain energy. Therefore, atomistic simulations are generally used to model the phenomena near the dislocation core. To circumvent this limitation, Lubarda and Markenscoff [2] have developed a variable core model that eliminates the stress singularity at the dislocation core. This is accomplished assuming that the displacement discontinuity is achieved gradually over some distance so that an edge dislocation is modelled as a doublet of two wedge disclinations before the limit between them is taken to zero. To implement this concept in a finite element scheme, we first model purely rotational crystal defects considering an appropriate pseudo-temperature distribution, which produces a dislocation array of increasing width. Accordingly, we model a discrete edge dislocation of linearly increasing width. Generally, any nonlinear increase of the displacement discontinuity may be also studied (Somigliana dislocations). This description of dislocation core is closer to experimental observations and has a physically anticipated behaviour reproducing the Volterra dislocation. Also, the obtained expression for the dislocation strain energy is bounded and can therefore be used as a measure of convergence. Further, we study interactions of variable core dislocations with free boundaries and coupled dislocation partials. In all cases, we recover the analytical solutions [3] for the stress distributions and the total strain energy and contribute with new results for anisotropic crystals.

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