Atomistic reconstruction of dislocation sets based on tensor algebra of lattice distortion fields

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Atomistic models of dislocations are often obtained by means of elastic-plastic relaxation of a perfect crystal lattice subjected to external loading. Another method, widely used in ab-initio modeling, is based on insertion of single dislocations into the perfect lattice. In such a case, the analytic formulas for displacement vector field inserting a single dislocation into elastic continuum are used. As of yet, the methods mentioned above do not give possibility for emerging the atomistic models of arbitrary chosen networks of dislocations. Among others, this problem concerns reconstruction the sets of dislocations observed by means of high resolution transmission electron microscopy. In this talk we discuss a deterministic method of obtaining atomistic models of dislocation networks. The method is based on a tensor algebra of elemental lattice distortion tensor fields used to subsequent insertion of single dislocations into deformed crystal lattice.

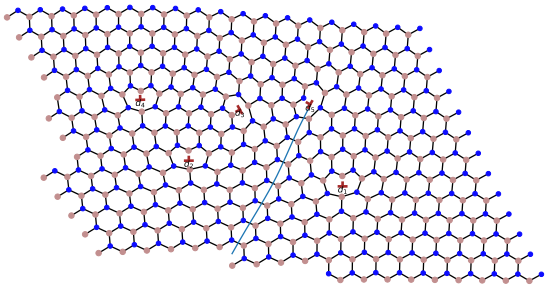

Figure 1. Preprocessed GaN lattice and glide plane along which the 5-th dislocation has been inserted[1].

Contrary to the linear-strain and linear-rotation measures, a lattice distortion tensor is the correct tensor measure of finite deformation. Thus, many different tensor fields of finite strain and finite rotation can be extracted uniquely from such a distortion field [2]. This enables a preprocessing of atomistic models of dislocations in terms of finite deformation approach. A method presented here links: (i) the analytic formulas for lattice distortions derived from the linear theory of dislocations, (ii) a tensor algebra of distortion fields, and (iii) the atom-by-atom reconstruction of a network of dislocation cores into crystal lattice (see Fig. 1). Configurations of atoms obtained in this way satisfy the stress equilibrium condition in terms of the linear theory of elasticity. On the other hand, the spatial Burgers vectors of dislocations are stretched and rotated to each other according to the finite deformation theory. Such obtained the resultant network of dislocations can be used next as the input data for the ab-initio and/or molecular dynamics programs to find a low energy configuration of atoms corresponding to a given interatomic potential.

[1] P. Jarosik, WURTZITE, https://github.com/pjarosik/wurtzite.

[2] P. Dłużewski K. Naplepka, *CAMES* **32**(4), 367-383, 2025. https://doi.org/10.24423/cames.2025.1963.