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Stabilization of free-standing GaN foils by threading edge dislocations ROMAN GRÖGER, Institute of Physics of Materials and CEITEC IPM, Academy of Sciences of the Czech Republic, LUCIEN LECONTE, Université Lille 1, France — Computational studies of core structures of $1/3[11\bar{2}0]$ threading edge dislocations in bulk GaN predict the existence of a 5/7-atom ring configuration when viewed along the [0001] direction. While this agrees with recent high-resolution electron microscopy observations, previous studies also reveal the existence of an 8-atom ring configuration. We employ molecular statics calculations to show that the core stability of the threading edge dislocation in free-standing GaN foils depends on the foil thickness and the terminations of their surfaces. For the foil thickness above 6 nm, the edge dislocation is predicted to possess the 5/7-atom ring core structure. However, with decreasing thickness and depending on surface terminations the minimum energy core structure may change to both 8-atom ring and 4-atom ring configurations. By quantifying the interaction energy of the dislocation with the surface of the foil, we show that there exist conditions for which the threading edge dislocation in the foil is more stable than in the bulk.

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