Analysis of nearly planar defects using the Thomas–Fermi–von Weiszäcker model

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ABSTRACT

We propose a well-posed minimization problem within the framework of the Thomas-Fermi-von Weiszäcker (TFW) model for computing the relative energy of nearly planar volume defects with respect to a perfect crystalline configuration. The typical geometry of the defective region is a thin film sandwiched between two perfect crystals of identical orientation. Assuming periodicity along the in-plane directions of the defect and symmetry along at least one in-plane direction, we build on prior analytical work on the thermodynamic limit of periodic supercell models in the TFW setting [1] and specialize it to the analysis of nearly planar defects. As an application of our theory, we establish the finiteness of the stacking fault energy for slip along a periodic direction within the framework of the TFW model. We also perform numerical simulations to compute the energy of the stacking fault defect and the electron density distribution using the minimization problem, and compare it with corresponding results obtained using high-fidelity orbital-free density functional theory (OFDFT) solvers. Finally, based on theoretical results on the decay properties of the electron density and potential, we propose a class of efficient numerical solvers for studying defects using general OFDFT models and illustrate its utility by computing the energies of surface defects in crystalline materials.

References

[1] Cancès, E.; Ehrlacher, V. Local Defects are Always Neutral in the Thomas–Fermi–von Weizsäcker Theory of Crystals. *Archive for Rational Mechanics and Analysis* **2011**, *202*, 933–973.