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On the interaction of dislocations with phase boundaries: theory and modeling with the phase field method

M. Budnitzki[†,1] **and S. Sandfeld**[†,2]

[†] Institute for Advanced Simulation (IAS-9: Materials Data Science and Informatics), Forschungszentrum Jülich GmbH, 52428 Jülich, Germany, https://fz-juelich.de/ias/ias-9
[1] m.budnitzki@fz-juelich.de
[2] s.sandfeld@fz-juelich.de

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In classical elasticity theory the stress-field of a dislocation is characterized by a $1/r$-type singularity. When considered together with an Allen-Cahn-type phase-field description for microstructure evolution, this singularity leads to an unbounded driving force acting on the order parameter. This results in non-physical predictions for the interaction between dislocations and planar defects like phase-, twin- or grain-boundaries. First strain gradient elasticity regularizes the dislocation core [1]. We developed a framework [2] that consistently couples first strain gradient elasticity to Allen-Cahn-type phase evolution. It is shown that the use of a strain energy density that is quadratic in the gradient of elastic deformation results in a non-singular stress tensor but may result in a singular driving force. However, a strain energy that is quadratic in the gradient of the full deformation tensor regularizes both the stress and the driving force for the order parameter, which makes it a more suitable choice. The applicability of this framework is demonstrated using a comprehensive example.

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