

Extended finite element with strain smoothing and level set method for predicting equilibrium shapes of nano-inhomogeneities

Xujun Zhao (1), Jianmin Qu (1) and Stéphane P.A. Bordas (2)

(1) Northwestern University, Evanston, IL USA 60208

(2) Cardiff School of Engineering, Institute of Mechanics and Advanced Materials, Cardiff University, Queen's Buildings, The parade, Cardiff CF24 3AA, Wales, UK,
stephane.bordas@alum.northwestern.edu

Key Words: Smoothed extended finite element method; Level set method; Wachspress shape function; Interface excess energy; Equilibrium shape.

ABSTRACT

Interfacial energy plays an important role in equilibrium morphologies of nanosized microstructures of solid materials due to the high interface-to-volume ratio, and can no longer be neglected as it does in conventional mechanics analysis.

The present work develops an effective numerical approach by means of a hybrid smoothed extended finite element/level set method [1] to model nanoscale inhomogeneities with interfacial energy effect, in which the finite element mesh can be completely independent of the interface geometry.

The Gurtin-Murdoch surface elasticity model [2,3] is used to account for the interface stress effect as in and the Wachspress interpolants [4] are used for the first time to construct the shape functions in the smoothed extended finite element method. The XFEM had been used previously in [5] to model nano-inhomogeneities. Selected numerical results are presented to study the accuracy and efficiency of the proposed method as well as the equilibrium shapes of misfit particles in elastic solids. Refer to [6] for details.

The presented results compare well with those obtained from theoretical solutions and experimental observations, and the computational efficiency of the method is shown to be superior to that of its most advanced competitor. More detailed results are presented in [7].

REFERENCES

- [1] Bordas SPA, Rabczuk T, Nguyen XH, Nguyen VP, Natarajan S, Bog T, Quan DM, Hiep NV, Strain smoothing in FEM and XFEM, *Computers and Structures*, 88 (23-24) (2010) 1419-1443
- [2] Gurtin, M.E. & Murdoch, A.I., 1975 Continuum Theory of Elastic-Material Surfaces. *Archive for Rational Mechanics and Analysis* 57, 291-323
- [3] Gurtin, M.E., Weissmuller, J. & Larche, F., 1998 A general theory of curved deformable interfaces in solids at equilibrium. *Philos Mag A* 78, 1093-1109
- [4] Wachspress, E.L., 1975 A rational finite element basis. Academic Press, New York.
- [5] Yvonnet, J., Le Quang, H. & He, Q.C., 2008 An XFEM/level set approach to modelling surface/interface effects and to computing the size-dependent effective properties of nanocomposites. *Comput Mech* 42, 119-131.(DOI 10.1007/s00466-008-0241-y)
- [6] Zhao, X.J. & Qu, J., 2012 Effects of interfacial excess energy on the elastic field of a nano-inhomogeneity. *Mech Mater* 55, 41-48.(DOI 10.1016/j.mechmat.2012.07.008)
- [7] Zhao, X.J., Qu, J., and Bordas, S.P.A. 2013 Effects of elastic strain energy and interfacial stress on the equilibrium morphology of misfit particles in heterogeneous solids *Journal of the Mechanics and Physics of Solids in press*