Free surfaces of crystalline nanostructures within a coarse-grained atomistic description

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A main characteristic of nanoscale structures is a large ratio of surface area to volume. Since the mechanical properties of a material body close to a free surface are different from the ones in the bulk of the material, the modelling of nanostructures must account for surface related effects. Standard approaches exhibit major drawbacks. Molecular simulations based on appropriate interatomic potentials can achieve high accuracy but the computational burden of fully atomistic resolution may become prohibitive. Continuum models in contrast, which accurately represent bulk material behaviour, fail to account for the effect of surface stresses without further modifications introducing a length scale dependence. This contribution aims to achieve predictive simulations of free surfaces of crystalline solids. The present modelling approach is a 3d fully nonlocal quasicontinuum method, [1], which belongs to the family of concurrent multiscale methods. The method's key feature of coarse-grained atomistics with adaptive resolution largely determines its accuracy and efficiency. Representative numerical tests assess the present method.

References

[1] Eidel, B., Stukowski, A. A variational formulation of the quasicontinuum method based on energy sampling in clusters, Journal of the Mechanics and Physics of Solids, 87, 203, 2009.