Configurational forces in crytal systems

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ABSTRACT

The concern of this work is to present the application of configurational mechanics in the context of atomistic fracture mechanics. In this concern, two and three-dimensional crystalline models including lattice defects are simulated to study configurational forces. Configurational forces are related to the integrity of material structure and the evolution of defects and phase interfaces under external loading.

We consider the configurational mechanics of atomistic systems as outlined in the first part of Steinmann's work (1991). Herein, the numerical treatment is done through the minimization of total potential energy that is calculated from Lennard-Jones interatomic energy. Subsequently, the derivative of energy with respect to interatomic stretch renders the atomistic configurational force. This stretch connects the interatomic spatial position to its material counterpart such that the configurational force indicates the change of interatomic position, particularly in the defect vicinity .

As a result of numerical examples, we obtain the atomistic configurational forces for crystal systems with cracks. In fact, these forces are computed in a post-processing step. The propagation of crack is captured entirely through atom-wise configurational force that can be interpreted as the driving force of crack growth.

REFERENCES

[1] Paul Steinmann, Sarah Ricker, and Elias Aifantis. *Unconstrained and cauchy-born- constrained atomistic systems: deformational and configurational mechanics*. Archive of Applied Mechanics, (1991) **81(5)**:669–684.