A STATIC ANALOG OF MOLECULAR DYNAMICS METHOD FOR CRYSTALS

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A new method of molecular statics based on independent displacements of atoms converging to an equilibrium state is proposed. The method is an attempt to combine the efficiency of Molecular Stratics (MS) to study fracture processes and the ability of Molecular Dynamics (MD) to minimize energy by independent motion of individual atoms. The method is demonstrated on a 2D imperfect crystal in which the interatomic pair-wise forces are governed by the Lennard-Jones potential. Accordingly, the equilibrium state of a lattice subjected to a boundary displacement is found through an ordered sequence of minimization steps. At each step the unbalanced resultant forces acting on each atom are found. Then each atom is moved into the direction of the unbalanced force vector by the amount functionally dependent on the magnitude of this force. Thus, in its form, the method is analogous to the MD one. It allows studying fracture, crack nucleation and propagation, etc. without the computer time constraints associated with the time step in molecular dynamics. An iterative procedure leading to the global equilibrium with a prescribed accuracy will be described and some numerical results demonstrating its validity will be given.