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Computer simulation of tensile testing*

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Abstract. A brief overview of the molecular dynamics method, with emphasis on the work of Parrinello and Rahman, is presented. Molecular dynamics is a method for studying classical statistical mechanics of well-defined systems through a numerical solution of Newton's equations. A set of N particles with coordinates r_i ($i = 1, \ldots, N$) and confined in a cell are allowed to interact through a potential. The bulk is usually simulated by periodically repeating the cell in space. Newton's equations are then solved numerically and the statistical averages of dynamical properties are calculated as temporal averages over the trajectory of the phase space. This method has already been used to simulate a liquid. Now, based on a Lagrangian formulation, it is possible to study systems under the most general conditions of externally applied stress. Unlike the earlier calculations, in this procedure, shape and size are governed by equations of motion obtained from the Lagrangian. Thus it allows us to study structural transformations which may be brought about by an interplay of external and internal stresses. By applying this technique to a single crystal of Ni, Parrinello and Rahman observe that the stress-strain relations obtained confirm with reported results. Under compressive loading it is found that Ni shows a bifurcation in its stress-strain relation and the system changes from cubic to hexagonal close packing. Such a transformation could perhaps be observed under extreme conditions of shock. Finally the scope of computer simulation is highlighted and the limitations of employing such a method are pointed out.

*only summary of the talk