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Particle modeling of dynamic fragmentation-I: theoretical considerations

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Abstract

This paper series adopts particle modeling (PM) to simulation of dynamic fracture phenomena in homogeneous and heterogeneous materials, such as encountered in comminution processes in the mining industry. This first paper is concerned with the setup of a lattice-type particle model having the same functional form as the molecular dynamics (MD) model (i.e., the Lennard–Jones potential), yet on centimeter length scales. We formulate four conditions to determine four key parameters of the PM model (also of the Lennard–Jones type) from a given MD model. This leads to a number of properties and trends of resulting Young's modulus in function of these four parameters. We also investigate the effect of volume, at fixed lattice spacing, on the resulting Young modulus. As an application, we use our model to revisit the dynamic fragmentation of a copper plate with a skew slit [J. Phys. Chem. Solids, 50(12) (1989) 1245].

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1. Introduction

Attaining a better understanding of the comminution of rocks, such as commonly taking place in the mining industry (e.g. [1]), is the primary motivation of the present study. Comminution involves complex crushing and fragmentation processes, which, from a basic engineering science perspective, are complex dynamic fractures of multi-phase materials. Thus, there is a need to simulate such processes from basic principles. The first tool that comes to mind is the continuum-type dynamic fracture mechanics. That approach, however, is well suited for analysis of well defined boundary-initial-value problems with simple geometries,

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Nomenclature

F_a	interaction force ($F = -G/r^p + H/r^q$) per pair atoms	q_a	exponential parameter in atomic structure
ϕ_a	interaction potential energy ($\phi = -\int F dr$) per pair atoms	m_a	mass of each atom (g)
G_a	parameter G in atomic structure	i max	total quasi-particle number in x–direction
H_a	parameter H in atomic structure	j max	total quasi-particle number in y–direction
S_a	stiffness $S_0(=(\mathrm{d}^2\phi/\mathrm{d}r^2)_{r=r_0})$ in atomic structure	k max	total quasi-particle number in z–direction
E_a	Young's modulus ($E = S_0/r_0$) in atomic structure	A	length of material specimen (cm)
r_a	equilibrium position in atomic structure, e.g., 2.46 Å for copper	B	width of material specimen (cm)
p_a	exponential parameter in atomic structure	C	height of material specimen (cm)

e.g. [2]. When more complex shapes are involved, numerical methods based on this approach—usually involving finite element methods—are necessary, and, with increasing problem complexity, tend to be unwieldy. Thus, when multiple cracks occur in minerals of arbitrary shapes with complex and disordered microstructures, yet another method is needed. To this end, we propose here a powerful modeling technique involving a uniform lattice discretization of the material domain, providing the lattice spacing is smaller (or much smaller) than the single heterogeneity of interest, e.g. [3,4]. The heterogeneity is, say, a gold particle, whose liberation from the mineral is of major industrial interest in the fragmentation process. While the case of quasi-static fracture/damage phenomena was researched in the past decade, the intrinsically dynamic comminution requires a fully dynamic lattice-type model with nonlinear constitutive responses.

In this paper series we adopt the so-called *particle modeling* (PM), developed by Greenspan [5–8] as an alternative to computational continuum physics methods in problems which become either hopelessly intractable or very expensive (time consuming) in atomistic and multi-scale solid and fluid systems. Since the method has its roots in molecular dynamics, it is sometimes called *quasi-molecular modeling* or *discrete modeling*. In essence, particle modeling is a dynamic simulation that uses small discrete solid physical particle (or quasi-molecular particles) as a representation of a given fluid or solid.

The two basic rules in the model set-up on larger-than-atomistic-scales are the conservation of mass and the conservation of equilibrium energy between the quasi-particle system and the atomistic material structure. Interaction between any two neighbors in PM involves a potential of the same type as the interatomic potential—here typically one of a Lennard–Jones type. Particle modeling can handle very complicated interactions in solid and fluid mechanics problems, also with complicated boundary and/or initial conditions; an example of the latter is the dynamic free surface generation in solids' fracture. In fact, due to these advantages, particle modeling has recently found increasing use in mineral and mining research especially in the studies of tumbling mills [9,10].

Research of the existing literature in PM shows that the following questions still remain open:

1. How does the choice of parameters in the interaction potential affect the resulting Young modulus and the effective strength of the material to be modeled?
2. How does the choice of volume of the simulated material, at fixed lattice spacing of quasi-particles, affect the resulting Young modulus?