MULTISCALE SIMULATION FOR HIGH ENERGY CLUSTER IMPACTS AND INDUCED DAMAGE

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ABSTRACT

We propose a new multi-scale simulation scheme which seamlessly combines the conventional molecular dynamics (MD) with the continuum mechanics formulated under the material point method (MPM). In MPM, modified interpolation shape functions are adopted to reduce artificial forces on the background hierarchical grids. The multi-scale method is validated using the example of wave propagation within a bar. The method is applicable to several kinds of potentials including the Lennard-Jones, EAM and a bonding-angle related potential for silicon. Examples of high energy Cu-Cu and Si-Si cluster impact are presented. The kinetic energy of the cluster is the critical process parameters. The evolution of displaced atoms is found to depend on the underlying lattice structures. For the case of Cu-Cu cluster impacts, stacking faults play an important role. The displaced atoms, visualized in the method of " local crystalline order" , propagate in an anisotropic manner. This implies the anisotropy in energy transformation process through impacts with multi interactions among cluster and surface atoms. With the help of the present multi-scale scheme, the computation capacity implemented in a personal computer could reach a system composed of 900 millions atoms. The case of Si-Si cluster impacts is also examined where the damage spreads in a more isotropic manner. For the case of cluster impact on a beam with pre-existing cracks, the high energy impact may seal the crack with amorphous matters and induces an efflux of atoms ahead of the crack mouth.

1. INTRODUCTION

Many physical phenomena, such as crack propagation, turbulence, and high energy cluster impacts, occur in multiple length scales, that is different length scales interact strongly to produce resulted complex behaviors. These phenomena pose notorious difficulty in computation. Atomistic and continuum simulations were combined to bridge the diverse length scales [1-3]. Here we add to this practice by advocating a new multiscale method that seamlessly handshakes the MPM and conventional MD method. The process of high energy cluster impacts inherently involves complex and multidimensional deformations, produces high pressure, temperature and shock waves as well as results in melting or even evaporating [4]. During the process of impacting, atoms near the impingement site are seriously distorted to different kinds of structures, and they can even be squeezed to the very proximity with each other. Energized atoms can have much higher velocity, escape the bondage of the substrate and flee away as

monomers and small clusters which results in a melting crater. We use conventional MD to model this highly distorted region. A reliable embedded-atom method (EAM) potential [5] is adopted in the simulation. The potential is suitable for modeling surface sputtering and shock waves, and has an improved reliability in atomistic simulations involving short atomic spacing and different atomic configurations. Leaving away from the impingement site, atoms still keep vibrating near ideal lattice sites and only elastic deformation occurs. We use MPM to handle this continuum region. The MPM/MD handshaking scheme is proposed here to model the high challenging phenomena.

2. MPM/MD HS SCHEME

2.1 The material point method (MPM)

MPM has been developed recently as a numerical tool for solving problems in solid dynamics. The conservation equation of linear momentum is solved on the background regular structured grid which enables computational techniques such as dynamical adaptive meshing [6]. The combination of Lagrangian and Eulerian schemes makes MPM suitable for solid dynamic mechanics problems including those with large deformations and those involving materials with history dependent properties such as plasticity or viscoelasticity. In MPM, modified interpolation shape functions are adopted to reduce artificial forces on the background hierarchical grids.

2.2 The handshaking of MPM/MD

We choose EAM potentials as an example to illustrate the MPM/MD handshaking method. It can be simply reduced to others potentials, such as Lennard-Jones potential suitable for noble gases and Stillinger and Weber (SW) potential for silicon which including two-body and three-body interactions. The method described here spatially divides the physical system into the MPM and the MD regions as illustrated in Fig. 1. An imaginary surface (interface) is drawn between the MPM and MD regions. Within twice the EAM potential cutoff from the interface, material points are located exactly at the ideal lattice sites. Within this region, material points are viewed as atoms but they move under the discrete momentum equation of MPM. The density of electron cloud is assigned to each material point under the EAM formulation. The material points in region II, within the range of electron cutoff from region I, serve to provide electron density for the material points in region I. The material points in region I, within the EAM potential cutoff from the interface, on the other hand, supply not only the electron density, but also the pair, triple and many body interactions with the atoms in the MD region. At each time step, forces on atoms applied by material points are calculated. The forces are then applied on material points according to the Newton's third law. These forces serve as boundary forces applied on material points. Thus the MD and MPM regions decouple, and evolve under their governing equations concurrently. Seamless handshaking can be obtained provided elastic constants in the MPM region matching those in the MD region.

Leaving the handshaking region, material points are enlarged to represent many atoms, rendering the computational efficiency of MPM. We use the hierarchical background mesh. All the simulations here are three dimensional. For bulk materials, the background mesh can be enlarged in three directions, i.e. eight elements condense to one big element. Material points are enlarged proportionally since the material is homogenous. The enlargement results in missing degrees of freedom. As the background mesh size

increases, some short wavelength phonons are not supported by the coarse mesh. The largest spacing depends on the shortest wavelength phonons expected to propagate unimpeded in the MPM region.

The handshaking scheme proposed here is a force-based connection which avoids assigning different kinds of weights of the contribution energy to Hamiltonian in the handshaking region [7]. Thus the method is suitable for different kinds of potentials including EAM potentials which include many-body interactions. Also the force-based connection is more flexible thanthe one-to-one displacement connection which causes artificial blocking against dislocation transition. Using proper method [8], one can achieve a defect permeable MPM/MD handshaking scheme.

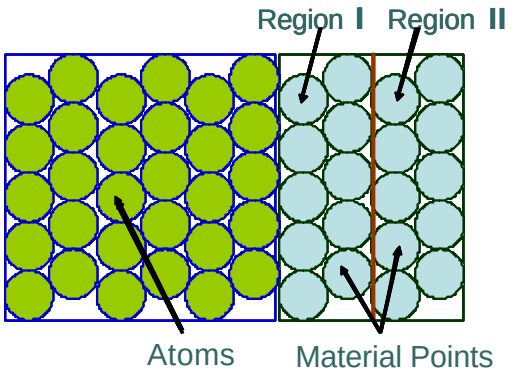


Figure 1 A schematic view of MPM/MD handshaking method. Material points in the handshaking region serve to provide an atmosphere for the atoms within the potential cutoff from the interface.

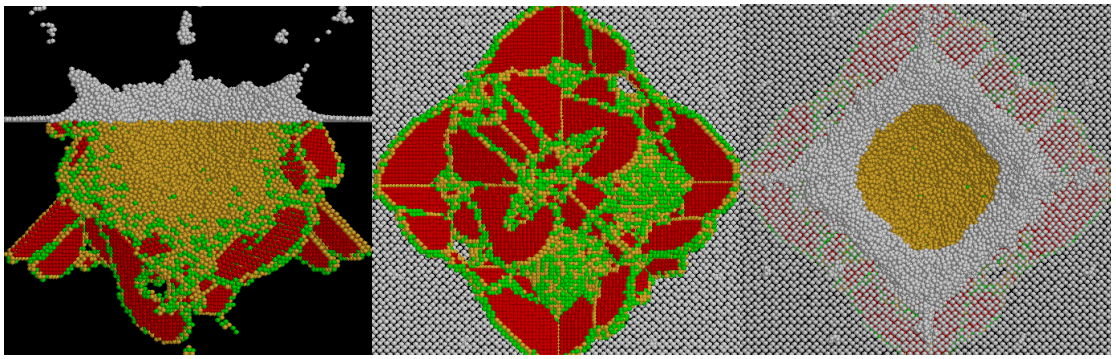
3. HIGH ENERGY CLUSTER IMPACTS

An application of this multiscale method is high energy cluster impacts. We simulate normal impacts of clusters flying with a velocity of 10km/s. Clusters are formed from spherical cutoff of an FCC lattice. Before simulation clusters are placed symmetrically above the target surface, which is taken as (0, 0, 1) plane. The top surface of the single crystal substrate is kept free and the rest five surfaces are fixed throughout the simulation. The time step isselected to ensure that the changing of atom positions at one step is at least one magnitude smaller than equilibrium atom spacing. The initial temperature is zero but is allowed to evolve freely. For all the cases the simulation time is 10ps. For 1052 atoms cluster impacting, the target is represented by a slab of dimension $277.6\times277.6\times138.8\ nm^3$, containing over 2.3 million atoms and 0.5 million material particles. If the total region is presented by atoms, about 900 million atoms are needed. Materials particles are arranged in 5 hierarchical layers, with each particle in the outside layer condensates 8 particles (binary condensation in each direction) of the inner layer.

The visualization of impacted atomistic system requires the identification of displaced atoms. Here for Cu it is defined as an atom whose structure, in terms of the "local crystalline order" [9-10], is altered to a non-FCC structure. Different colors are assignedto different structures to provide a clear image of defects: atoms with local FCC order are colored transparent, atoms on and above target surface are colored white, atoms with local HCP order are colored red, atoms with other 12-coordinated combinations are colored green, and atoms with none 12-coordinated combinations are colored yellow. For Si, displaced atoms are defined as those with none 4-coordinated atoms and colored green. Surface atoms are also colored white.

The graphs in Fig. 2 give snapshots of impacting for clusters with 1052 atoms. First damage spread out almost in an isotropic manner. Then the disordered atoms prefer to propagate along the four closed packed {111} planes. Disordered atoms on different slip planes interact with each other and then prefer to propagate along the four interaction directions ($[0\bar{1}\bar{1}]$, $[01\bar{1}]$, $[10\bar{1}]$ and $[\bar{1}0\bar{1}]$ as illustrated in Fig. 2 (a-c)). Dislocation loops can be observed in Fig. 2 (a). Thus the common slip directions of interacted slip planes are displaced atoms' most favorable propagation paths.

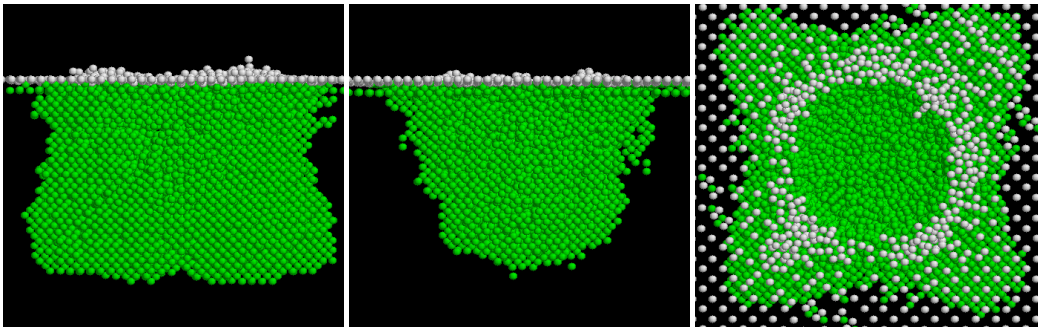
The evolution of crater shapes also indicates that the FCC lattice structure plays an important role in the impact process. The top view of craters evolves from a circle to a square (Fig. 2 (c)). The crater first deforms uniformly, corresponding to the isotropic propagation of displaced atoms. Then the deformation rate is higher in <100> and changes the top view of the crater to a square, corresponding to the displaced atoms preferring to propagate along slip planes' interaction directions. It is the burst of stacking faults that makes the deformation rate higher in <100> which changes the shape of the crater from a circle to a square.



(a) (b) (c)

Figure 2 (a)Frontal views of local crystalline orders for 4.2ps after impact for the cluster with 1052 atoms .(b) and (c)The corresponding bottom and top view of graph (a).

For the purposes of comparison, Si clusters impacting with a Si substrate is also simulated. We adopt the potential proposed by Lenosky et al [11]. That potential combines the SW formulation and the EAM form, and is identical to the modified EAM (MEAM) form. The potential provides a reasonable description for the energetics of all atomic coordination numbers and accurately predicts formation energies and geometries of interstitial complexes, small clusters and interstitial-chains. It can be seen that more damage occurs in $[110]$ and $[1\bar{1}0]$ directions (Fig. 3 (a) and (c)), which is quite distinct from that of Cu cluster impacting on a Cu substrate as illustrated in Fig. 2. The top view of the crater is always a circle (Fig. 3 (c)). At the late stage of impact, the target recovers to an almost isotropic profile (Fig. 3 (b)) while for Cu-Cu impacting stacking faults burst and make the displaced atoms anisotropic.



(a) (b) (c)

Figure 3 (a-b)Frontal views of local crystalline orders at 1.3ps and 2.5ps after a Si cluster of 260 atoms impacting with a Si substrate. (c)The corresponding top view of graph (a).

4. INTERACTION BETWEEN CRACKS AND CLUSTER IMPACTS

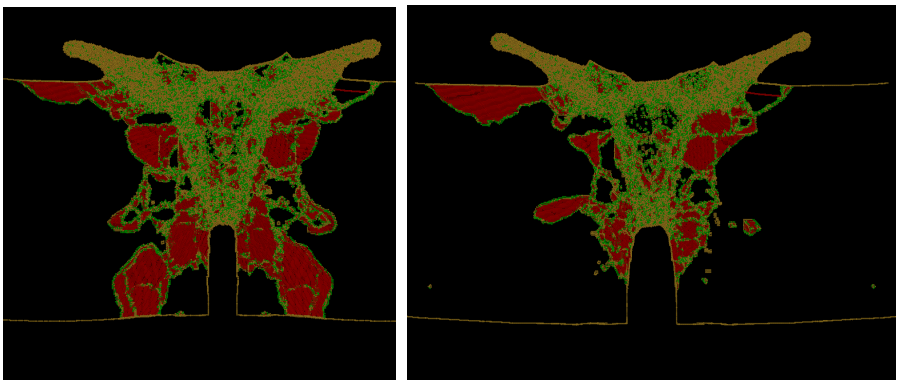


Figure 4 Local crystalline orders at 15.0ps (left) and 20.8ps (right) after impact.

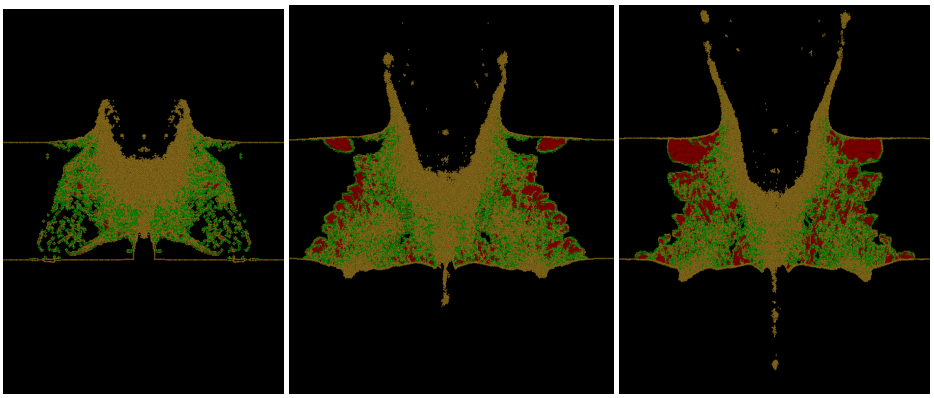


Figure 4 Local crystalline orders at 2.5ps (left), 5.0ps (center) and 7.5ps (right) after impact.

We use this approach to observe the interaction between cracks (under mode I or mode II loading) with the cluster impacts. The clusters are impacted on a beam of length 347.6nm and thickness 2.9nm. For mode I case, the simulation depends critically on the parameters such as the beam height H, the impacting velocity v and the size of the cluster L. Figure 4 delineates the cluster impact on a beam with H=34.7nm, v=2km/s, N=51200. The relative large size of the impacted causes the crack to blunt. Figure 5 shows another case with H=17.4nm, v=10km/s, N=2048. The kinetic energy of the impacting cluster is exactly the same as the previous case, but the beam height is reduced to a half. A different deformation pattern is observed. The crack becomes a guiding channel for the mass flow, and the atoms shoot out in terms of efflux ahead of the crack mouth.

5. CONCLUSIONS

We have developed a MPM/MD handshaking scheme which seamlessly combines the MPM and MD regions. The method is seamless and is applicable for pair, triple and many-body potentials. Using the MPM/MD handshaking method, we study high energy Cu-Cu and Si-Si cluster impacts. The lattice structure is found to play an important role in the deformation process.

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