RECENT ADVANCES IN DEVELOPING THE GENERALIZED INTERPOLATION MATERIAL POINT METHOD FOR SIMULATING BRITTLE FRACTURE BASED ON MOLECULAR DYNAMICS

Jun Tao¹, Shan Jiang², Yu-Chen Su³ and Zhen Chen⁴

¹ State Key Laboratory of Structure Analysis for Industrial Equipment, Department of Engineering Mechanics, Dalian University of Technology, Liaoning, China 116024; Email: taojun@mail.dlut.edu.cn
² Department of Mechanical Engineering, University of Mississippi, University, MS, USA 38677; Email: jiang@olemiss.edu
³ Department of Civil & Environmental Engineering, University of Missouri-Columbia, Columbia, MO, USA 65211; Email: vsdx8@mail.missouri.edu
⁴ State Key Laboratory of Structure Analysis for Industrial Equipment, Department of Engineering Mechanics, Dalian University of Technology, Liaoning, China 160024; Department of Civil & Environmental Engineering, University of Missouri-Columbia, Columbia, MO, USA 65211; Email: chenzh@missouri.edu

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ABSTRACT

Based on the recent research results on multiscale modeling and simulation of energetic composites under simple loading conditions [1, 2], an effort is being made to develop a hierarchical multiscale approach based on molecular dynamics (MD) and the generalized interpolation material point method (GIMP). Basic mechanical behaviors, such as elastic and damage responses to external loading conditions, are predicted at the molecular level using MD. The MD results are then employed to formulate an elastodamage model within the GIMP framework. The multiscale model-based simulation procedure is used to deal with large deformation and fracture. In this conference, recent computational results will be presented and future research tasks will be discussed based on the findings.

1 INTRODUCTION

Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) is a powerful nitramine high explosive [2,3]. The isothermal elastic properties of HMX were calculated by Sewell et al. [3] using atomistic simulations. Peng et al. [4, 5] used the electronic structure calculations to predict the crystal structures, elastic properties and the equation of state of β-HMX, which is the most stable standard ambient conditions among the three pure polymorphs of the crystalline HMX. These studies provided basic mechanical properties for developing constitutive models at continuum level. Recently, it is of interest to understand the macroscopic mechanical responses of energetic crystals in terms of fundamental elastic and inelastic deformation processes to better understand and predict the shock sensitivity. However, the need to incorporate the fundamental molecular-scale properties and processes into continuum level models motivates the development of multiscale methods. However, the multiscale methods to describe the mechanical behaviour for single-crystal HMX are still lacking, especially those to capture the nonlinear elastic and damage responses.

In the past decades, many multiscale methods were proposed to combine the molecular dynamics (MD) and the material point method (MPM) [6–8], where the MD simulations are used to provide details of the physical properties at nanoscale level and the MPM is employed to simulate the macroscopic responses such as the deformation, multiphase interaction and fracture at continuum level. Compared with the Finite Element Method and other mesh-based methods, the MPM, as a particle-based method, has advantages in simulating problems involving large deformation under extreme loading conditions [9, 10]. Although many multiscale methods that coupled the MD and MPM were proposed, many of
them were mainly focused on the simulations of metals and other simple crystal structures rather than low-symmetry, anisotropic crystal structures such as HMX and most other organic molecular materials.

In this study, a predictive constitutive model is developed for simulating the inelastic and damage responses of the β-HMX under external loading conditions using a hierarchical multiscale approach that combines MD and MPM, where the basic mechanical properties of the material are predicted using the MD simulation at molecular level, and the results are used to construct an elastodamage model that incorporates the anisotropy and nonlinear elastic-damage behaviour of the material. The generalized interpolation material point (GIMP) method [11], which is a generalization of conventional MPM formulation [12], is employed in the continuum calculations to reduce the numerical errors caused by the cell-crossing problem suffered in the original MPM.

2 RESULTS AND DISCUSSION

2.1 MD simulation of β-HMX

In MD simulations, three different supercell sizes were constructed by replicating the unit cell (Figure 1(a)) using lattice parameters, namely $5a \times 5b \times 5c$, $10a \times 10b \times 10c$ and $20a \times 20b \times 20c$ (Figure 1(b)). The MD simulations were performed using the LAMMPS code [13] with three-dimensional periodic boundary conditions. Basic loading tests, such as uniaxial tension along x, y and z and shear in the xy-, xz-, and yz- planes were performed. Figure 2(a) shows the results for the β-HMX subjected to tensile strain parallel to the y-direction with three different supercell sizes. The predicted nonlinear elastic-damage behaviour, peak limit and failure strain are practically independent of the supercell size. In Figure 2(b), it can be found that the unloading curves essentially follow the loading path back to the original point, even though small residual strains exist at the ends of the unloading simulations. Figure 3 shows the MD results for stress–strain curves for tension tests along y and z, and shear test on the xz-plane with atomic configurations at specific strains.

2.2 An elastodamage model for GIMP

Based on the MD results, a nonlinear elastodamage model for the failure of β-HMX is proposed for the GIMP simulations in continuum level. The secant tensor $E^{ed}$ is used to construct the stiffness matrix. According to the MD results, the main features of the nonlinear elastodamage for β-HMX can be captured even if inelastic flow prior to the onset of damage is completely neglected. Therefore, the strain-based constitutive equation for the elastodamage process can be simplified to $\sigma = E^{ed} : \epsilon$. The components $E^{ed}$ are obtained from the MD simulation using the following equation:

$$E^{ed}_{ij} = \begin{cases} \frac{\sigma_i}{\epsilon_j}, & 0 < |\epsilon_j| < \epsilon_j^p \\ 0, & |\epsilon_j| > \epsilon_j^p \end{cases}$$

where $i = 1,2, ..., 6, j = 1,2, ..., 6$ and $\epsilon_j^p$ is the peak strain.

2.3 GIMP results and discussion

The GIMP simulations at continuum level were performed using the MD-based constitutive model for a sample of β-HMX with monoclinic shape and edge lengths $A = 10^9a$, $B = 10^9b$, and $C = 10^9c$. A constant velocity $v = 100$ m/s parallel to the y-direction was applied to each face of the box, with the box lengths in the x- and z-directions held constant. Figure 4 shows the damage surfaces at $t = 4 \times 10^{-4}$ s from the GIMP simulations using two different peak strain values $\epsilon_j^p$. As a result, the damage surfaces form at the same location despite the different peak strain in the brittle-damage model. Thus the response of the material predicted by GIMP is not highly sensitive to the peak strain values. Figure 5 shows the comparison of the stress–strain relationships calculated from the GIMP simulation using the hierarchically based elastodamage model and the results from the MD simulations. It can be seen from the figures that the proposed constitutive model and the hierarchical multiscale approach are robust for predicting the mechanical responses with stable numerical results at continuum level.
Figure 1: (a) Molecular and unit-cell structure of β-HMX. (b) Depictions of the supercell systems.

Figure 2: Stress–strain relationships obtained from MD for tension tests along y (a) for different supercell sizes and (b) for loading and unloading from different applied strains.
Figure 3: stress-strain relationships from MD simulations with atomic configurations for (a) tension along y, (b) tension along z and (c) shear on xz plane.
Figure 4: Configurations of a GIMP sample showing the damage surface after failure. (a) and (b): the case of the maximum strain criterion $\varepsilon^p_2 = 0.15$; (c) and (d) the case of the maximum strain criterion $\varepsilon^p_2 = 0.23$.

Figure 5: Stress–strain relationship obtained from GIMP simulations and MD simulations and the smoothed MD results

3 CONCLUSIONS

A predictive elastodamage constitutive model was developed using a hierarchical multiscale approach that combined the MD and GIMP for simulating the mechanical response of the single-crystal $\beta$-HMX under simple loading conditions. The GIMP results predicted by the hierarchically obtained elastodamage model can get identical results with the MD simulations in stress-strain relationships and damage surfaces. However, this model is still in preliminary development and has limitations and drawbacks. Future research will be focus on the development of more general constitutive models such as elasto-plastic-damage model and bifurcation-based decohesion model, and more robust multiscale method for simulating the energetic materials including the $\beta$-HMX and other explosives.

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