Computational Materials Science 75 (2013) 73–78

Contents lists available at SciVerse ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Atomistic-to-particle multiscale coupling method for adiabatic shear banding simulation

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ARTICLE INFO

Article history:
Received 22 December 2012
Received in revised form 11 February 2013
Accepted 18 March 2013
Available online 6 May 2013

Keywords:
Atomistic-to-particle coupling method
Adiabatic shear band
Mixture criterion

ABSTRACT

An atomistic-to-particle (AtP) multiscale coupling method is proposed to study the initiation of adiabatic shear band (ASB) under shock loadings from both macro and micro aspect. A non-interpolation coupling technique is used to construct the atomistic boundary condition between micro and macro method, and atomistic contribution to internal force is also incorporated in the overlapping region. Combining with the mixture criterion of critical strain and temperature, this AtP method has been successfully applied to study the micro mechanism of ASB onset for hat-shaped metal sample. Multiscale simulation results at the time of ASB onset indicate that highly strain localization and rapid temperature rise are main reasons for ASB initiation. Numerical results are validated by experimental observations.

1. Introduction

Adiabatic shear banding under shock loadings is a complex procedure involving the interactions of multiple time and spatial scales [1–5], and continuum scale ASB failure has its micro origins, such as dislocation nucleation and phase transform. Multiscale numerical simulation that coupling micro molecular dynamics (MD) with macro finite element (FE) computation is an important tool for studying this procedure [6–12]. However, micro defects of material will always result in strain localization and fracture damage, which is a tough task for the mesh rezoning and adaptivity in FE computation. On the other hand, the meshfree methods (MM) that developed for dealing large deformation problems have been witnessed fast progress in recent decades [13–18]. These methods have been successfully used in the numerical simulations of shock loading problems, and attract widely research interests. There are several important landmark works in the study of ASB mechanism with MM methods by Li and cooperators [19,20]. Mesh alignment sensitivity is greatly reduced, and the ductile-to-brittle failure mode transition of ASB has been successfully demonstrated in numerical simulations [19], which coincides with experimental observations. New dynamic microstructures in ASB, such as periodic fluctuation and oscillatory pattern of temperature and the thermo-mechanical instability, are revealed from the simulation [20]. In addition, the effects of dynamic microstructures on ductile failure mechanism is also discussed, and its recent developments in thermo-mechanical simulations are reported [21]. In 2007, Gu et al. presented a transition algorithm to combine particles and atoms, and the effect of different transition region sizes and transition particle numbers is discussed [22].

There are special difficulties in the study of atomistic-to-particle (AtP) coupling methods. Besides their own characteristics of particle methods including the complexity in basis function construction and numerical integration, new difficulty exists in the computation of AtP boundary condition and internal particle force. We propose an AtP coupling method in this paper, and focus on the following two points. First, a non-interpolation coupling technique is used to construct the atomistic boundary condition. The meshfree basis functions in overlapping region are calculated by incorporating neighboring atomistic information, and the approximate integration scheme of time history kernel function is presented. Second, based on the critical strain and critical temperature criterion, the mixture ASB onset criterion is used in the numerical simulation. Combining with experimental results, the micro mechanism of ASB initiation is discussed. Section 1 is the introduction, Section 2 introduces the AtP multiscale coupling method, including the construction of atomistic boundary condition and computation of basis functions in overlapping region. Experiment and physical model is presented in Section 3, with analysis of numerical simulation results, and Section 4 summaries this paper.

2. Atomistic-to-particle coupling method

2.1. Governing equation

Ω_0 and Ω are open sets in $\mathbb{R}^N$. The deformation

$$\begin{cases} \varphi : \Omega_0 \to \Omega = \varphi(\Omega_0), \\ \mathbf{X} \mapsto \mathbf{x} = \varphi(\mathbf{X}, t), \qquad \forall \mathbf{X} \in \Omega_0, t \geqslant 0. \end{cases} \tag{1}$$

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http://dx.doi.org/10.1016/j.commatsci.2013.03.036

maps the initial position X to current coordinate x.

The deformation gradient, deformation Jacobian determinant is defined as

$$\mathbf{F} = \nabla_{\mathbf{X}}\varphi, F_{iK} = \frac{\partial \varphi_i}{\partial X_K} = \frac{\partial x_i}{\partial X_K}, \quad J = \det(\mathbf{F}).$$

The governing equation is the conservation law of mass, momentum and energy:

$$\begin{cases} \dot{\mathbf{u}} = \mathbf{v}, \\ \rho J = \rho_0, \\ \rho\dot{\mathbf{v}} = \rho\mathbf{b} + \nabla_x \cdot \sigma, \\ \rho\dot{\epsilon} = \rho r + \nabla_x \mathbf{v} : \sigma + \nabla_x \mathbf{q}. \end{cases} \tag{2}$$

where ∇_x, $\nabla_x\cdot$ are the gradient and divergent operators of current configuration, and $\dot{\mathbf{u}}, \dot{\mathbf{v}}$ and $\dot{\epsilon}$ means Lagrangian time derivative. $\mathbf{u} = \mathbf{x} - \mathbf{X}$ denotes the displacement vector, ρ_0 and ρ are the initial and current density. $\mathbf{v}$,$\mathbf{b}$, σ, r and $\mathbf{q}$ are velocity, body force, Cauchy stress tensor, energy source term and heat flux, respectively. The energy is measured per unit mass, and the total energy is defined as

$$E = \epsilon + 0.5\mathbf{v}^2,$$

where ϵ is the internal energy.

$\sigma^T : \nabla_x \mathbf{v} = \sigma_{ji}\partial_{x_i} v_j$, since σ is symmetric, $\nabla_x \mathbf{v}{:}\sigma = \sigma{:}\nabla_x \mathbf{v} = \sigma^T{:}\nabla_x \mathbf{v}$. The variational form of Eq. (2) can be written as:

$$\begin{cases} \int_\Omega \delta\psi_\gamma(\rho_0 - \rho J)d\Omega = 0, \\ \int_\Omega \delta\psi_\kappa \cdot (\rho\dot{\mathbf{v}})d\Omega + \int_\Omega \nabla_x^s \delta\psi_\kappa : \sigma\, d\Omega - \int_\Omega \delta\psi_\kappa \cdot (\rho\mathbf{b})d\Omega = 0, \\ \int_\Omega \delta\psi_\gamma \cdot (\rho\dot{\epsilon})d\Omega - \int_\Omega \delta\psi_\kappa \left(\nabla_x^s \mathbf{v} : \sigma + \nabla_x \cdot q + \rho r\right)d\Omega = 0. \end{cases} \tag{3}$$

where $\nabla_x^s = \frac{1}{2}\left(\nabla_x^T + \nabla_x\right)$ is the symmetric part of the gradient operator, $\nabla_x \mathbf{v} : \sigma = \nabla_x^s \mathbf{v} : \sigma$. Inserting the particle basis functions follows the discretization form of Eq. (2).

2.2. Atomistic-to-particle coupling

In this paper particle simulation is carried out over the whole domain, while MD simulation only exists in those critical regions, e.g., overlapping region Ω_{md}. Without point interpolation property in particle method, the key point of coupling particle method and MD simulation is to build the two-way interact mechanism.

Dynamical coupling including the issue of temperature effects. To ensure conservation of the total energy in this simulation, the energy flow into Ω_{md} from continuum region is balanced by the additional work done on MD system. We define the following temperature diffusion equation at each particle timestep Δt in Ω_{md}, with continuum temperature on Γ_{md} as boundary condition:

$$\begin{cases} \rho c_p \dot{T}(x,t) = \nabla \cdot \kappa \nabla T(x,t) \text{ in } \Omega_{md}, \\ -\mathbf{n} \cdot \kappa \nabla T(x,t) = \bar{q}(x,t) \text{ on } \Gamma_{md}. \end{cases} \tag{4}$$

where c_p, κ are specific heat and conductivity. $\bar{q}$ is heat flux on Γ_{md}, and continuum temperature is calculated from the convert of plastic work. To solve this problem, the standard finite difference scheme for diffusion equation is applied over an artificial uniform grid generated in Ω_{md}. With the temperature on each grid point, the neighboring atom velocities can be corrected if the system is at equilibrium (with zero mean velocity):

$$\frac{3}{2}nk_B T = \left\langle \sum_\alpha \frac{1}{2} m_\alpha |v_\alpha|^2 \right\rangle, \tag{5}$$

where k_B is Boltzmann's constant and the angle brackets denote an average of time for the system relax. This velocity correction is constrained by the following energy conservation condition:

$$\sum_\alpha \frac{m_\alpha}{2} \lambda_\alpha v_\alpha \cdot v_\alpha = \int_{\Gamma_{md}} \mathbf{n} \cdot \kappa \nabla T, \tag{6}$$

where $\lambda_\alpha v_\alpha$ is the corrected velocity, with λ_α as the scaling factor of atom α. The LHS of Eq. (6) denotes the additional work done to MD, while the RHS is the energy into Ω_{md}.

Next we introduce the non-interpolation coupling technique that used in our simulation. The ghost atoms are calculated from neighboring particles. The displacement of particle $\mathbf{u}$ can be represented by meshfree basis functions in Ω_{md} as: $\mathbf{u}^h = \sum N_I \mathbf{u}_I^h$, and MD displacement field satisfies the following motion equation:

$$M\dot{\mathbf{v}}_\alpha = f_\alpha^{ext} - f_\alpha^{int},$$

where f_α^{int} is calculated from the potential function $U(u)$ by using $f_\alpha^{int} = \nabla_u U(u)$, and f_α^{ext} is the external force vector. The parameters of time history kernel (THK) calculation is introduced in detail (see Ref. [23]). The ghost atoms are act as boundary condition of real atoms. To minimize the energy reflection at atomistic boundary, the motion of atom can be formulated as in [24]:

$$m\ddot{x}_i(t) = -\frac{\partial V}{\partial x_i} + \int_0^t d\tau \sum_{j=1}^N \beta_{ij}(\tau)\dot{x}_j(t-\tau) + \sum_{j=1}^N \beta_{ij}(t)x_j(0) + R_i(t) \tag{7}$$

Based on scale separation and linear decomposition assumption in [7], the potential energy term $-\frac{\partial V}{\partial x_i}$ at equilibrium positions is viewed as coarse scale, and the time-dependent memory kernel matrix $\beta(t)$ can be obtained by applying Laplace transformation in [10,23]. In this section, we study the approximate scheme of calculating integration term of THK function: $I_\beta = \int_0^t \sum_{j=1}^N \beta_{ij}(\tau)\dot{x}_j(t-\tau)d\tau$ without Kronecker-delta condition.

Inserting $\mathbf{v}_i^h = \dot{\mathbf{u}}_i^h, \mathbf{v}_\alpha = \dot{\mathbf{u}}_\alpha$ and $\dot{\mathbf{u}}_i^h = \sum \omega_k \cdot \dot{f}_k(x,t)$ follows

$$\begin{aligned} I_\beta &= \int_0^t \sum_{j=1}^N \beta_{ij}(\tau)(\mathbf{v}_i^h + \sum_\alpha \dot{\mathbf{u}}_\alpha)(t-\tau)d\tau, \\ &= \int_0^t \sum_{j=1}^N \beta_{ij}(\tau)\left(\sum \omega_k \cdot \dot{f}_k(x,t) + \sum_\alpha \dot{\mathbf{u}}_\alpha\right)(t-\tau)d\tau. \end{aligned} \tag{8}$$

At each particle time step Δt, inserting the above I_β into Eq. (7) for calculating ghost atom displacement $u_{\alpha,G}$. During the same particle timestep, this meshfree interpolation contribution is the same, while the prediction of acceleration of ghost atoms is a constant that interpolated from that of the particles. At each MD timestep δt, the boundary condition of MD simulation is defined by those ghost atoms. During each particle timestep Δt, the energy is conserved if Eq. (6) holds. With boundary condition and continuum temperature on Γ_{md}, MD simulations are carried out, and the velocity of atom is corrected by the additional force that results from energy balance. The average of RHS in Eq. (5) is taken over the relax time of MD system. Finally, the particles are corrected by using atomistic information, and the two-way interaction between continuum and atomistic models is included.

2.3. Internal particle force algorithm

In this section the calculation of macro internal particle force with atomistic information in Ω_{md} is introduced. As shown in Fig. 1, the ellipse $\mathcal{A}_K$ denotes the influence domain of particle K, and the dot line denotes the background integration cell, with $' \times '$ as the Gauss integration points. Above Γ_{md} is the macro particle region, and below the interface is Ω_{md} coupling MD and particle. Solid black dots are real atoms x_α, while hollow white dots are ghost atoms. Ghost atoms are used to construct the atomistic boundary condition, which is explained in the last section.

The calculation of internal nodal force f_K^{int} is the key for solving momentum equation and obtaining the acceleration of particles. It is well known that reduced integration will pollute numerical accuracy heavily, especially for interface elements. We adopt Lagrangian kernel function and high order Gauss quadrature