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Multiscale simulation of adiabatic shear bands initiation and propagation under impact loading

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ABSTRACT

A multiscale model which coupling finite element approach (FEA) and molecular dynamic (MD) was adopted to simulate the initiation and propagation of adiabatic shear bands (ASBs). In this model, FEA is based on the Johnson-cook plastic and damage model, the MD is based on the embedded atom method (EAM) potential. By FEA, the variation of temperature and stress fields during the initiation and propagation of ASBs was predicted, the effect of loading rate on the temperature and propagation rate of ASBs were also studied. Results of FEA, i.e. displacement and temperature were applied in MD to study the microstructure evolution at the early stage of ASBs. It was found that micro-crack and void initiation and propagation is the dominant mechanism, which is consistent with observation in experiment.

1. INTRODUCTION

Adiabatic shear bands (ASBs) are localized shear deformation regions which result from dynamic plastic instability for metals and alloys under impact, explosion and some other high strain-rate loadings. The widths of ASBs are usually only range from 10 micrometers to 100 micrometers, but the initiation and propagation of ASBs may induce unexpected failure and affect the dynamic mechanical properties.

The propagation of ASBs looks similar to the propagation of crack, but the physical background is much more complicated, so it is difficult to establish a physical sound model to simulate the initiation and propagation of ASBs. In recent years, quantitative description of adiabatic shear process was usually based on the so called thermo-visco-plastic constitutive model which takes the strain hardening, strain rate hardening, thermo softening effect into account and dynamic failure criterion which can predict the initiation and propagation of ASBs. Experimental study show that phase transformation, recrystallization, micro crack and void initiation and propagation were the main mechanism in ASBs(Xu 2008, Marchand 1988, Meyers 2001, Longre 2005), but the relation between micro-mechanism and macro-criterion still needs further research.

The initiation of ASBs is a transient process, which only last for a few micro seconds, so it is very hard to obtain the information such as temperature from experiment. In recent years, with the development of computational techniques, numerical simulation of ASBs becomes more and more popular. Finite element approach (FEA) which is one of the most mature methods is widely used in studying ASBs. Simulations of ASBs are usually based on constitutive model and failure criterion, some characteristics of the shear bands such as propagation velocity and temperature rise can be easily obtained(Zhou 1996, Li 2010). Since severe plastic deformation undergoes in localized region during adiabatic shear, Medyanik (2007) use meshless approach to simulate the large deformation effect and his failure criterion is based on recrystallization in shear bands experiments. Results such as shear band width, maximum speed and temperature are approximate to experiments results. Even though some of these numerical models are based on the physical mechanism, quantitative relation between these mechanisms and macroscale characteristics still need further study.

In this paper, a 2-D single-edge cracked finite element model based on Jonson-cook thermo-visco-plastic constitutive model and Jonson-cook damage model was established. High speed shear loading was applied on the upper and lower boundary of the model. Molecular dynamic model based on EAM potential was also established in crack tip region, i.e. ASBs initiation region. At the initiation stage of shear bands, FEA results, such as temperature and displacement, were passed to MD boundary to perform molecular dynamic simulation. By FEA calculation, macro-scale phenomena were obtain, by MD calculation the relationship between macro-scale phenomena and microstructure evolution was qualitatively revealed. At last, the effect of external factors, i.e. loading speeds were also systematical analyzed.

2. Numerical model

Intrinsically, materials deformation and failure is the results of dislocation emission, twinning and micro crack and void initiation and propagation on micro-scale, so it is incomplete to study materials deformation and failure only with phenomenological damage parameters and criterions. The initiation and propagation of ASBs is multi-scale phenomenon which span macro-scale, meso-scale, micro-scale, so a multi-scale approach was proposed to study the macro-process and micro-process of formation ASBs.

Multiscale model coupling MD and FEA was shown in Fig.1. In FEA region, 2-D plane stress elements were used and the total size of the model is 5mm X 4mm as shown in Fig.1 (a), a 1mm notch and a 0.26mm pre-crack were set on left side of the model. On the purpose of simplicity and verification, the FEA model size was similar to the size in ref. [6] which used meshless approach. The upper boundary was fixed, and a dynamic shear loading was applied on the lower boundary. The mesh form has a direct effect on calculating precision and time, to the improve the precision and save time, fine mesh was used in the vicinity of the crack and the expected shear bands, coarse mesh was used in other region. MD region is in the crack tip region, Fig.1 (b) show the detail of MD model, the size of it is 200nm X 50nm.

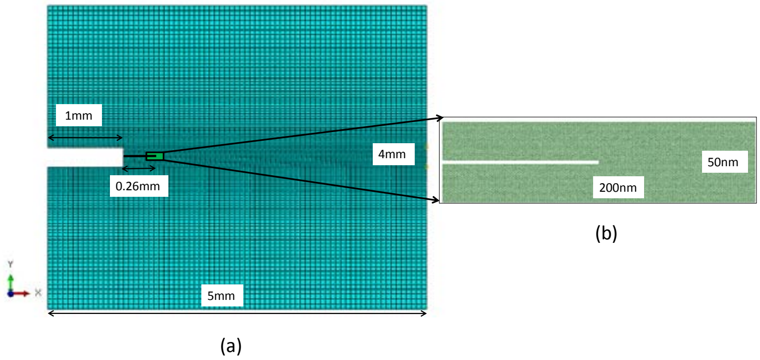

Fig.1 Multiscale model of shear sample, (a) FEA region, (b) MD region

Johnson-Cook constitutive model base on Von Mises yielding surface was used in continuum simulation, it can simulate strain hardening, strain-rate hardening and thermo softening effect at the same time, the relation between effective stress and effective plastic strain can be describe as follows:

$$\sigma = [A + B(\varepsilon^p)^n]\,[1 + c\ln(\frac{\dot{\varepsilon}^p}{\dot{\varepsilon}_0})]\,[1 - (\frac{T - T_r}{T_m - T_r})^m] \qquad (1)$$

Where A is yielding strength on quasi static condition, B and n are strain hardening coefficient and exponent respectively, C is strain-rate hardening coefficient, $\dot{\varepsilon}^p$ is reference strain rate which often assume as 1, m is thermo softening exponent, Tr and Tm are reference temperature and melting point.

To simulate material failure under mechanical loading, an accumulate damage model based on effective plastic strain was introduced, damage parameter for a specified element is:

$$\omega = \sum(\frac{\Delta\varepsilon^p}{\varepsilon_f^p}) \qquad (2)$$

When ω equal to 1, the element failed, $\Delta\varepsilon^p$ is the increment of effective plastic strain, ε_f^p is the effective plastic strain at failure. It is widely accepted that for most metals and alloys the forming of ASBs is under some specific condition, i.e. strains, strain-rates and temperatures. Here we use a plastic failure criterion (Johnson 1985) corresponding to Johnson-Cook constitutive model:

$$\varepsilon_f^p = [d_1 + d_2 e^{d_3(p/q)}]\,[1 + d_4\ln(\frac{\dot{\varepsilon}^p}{\dot{\varepsilon}_0})]\,[1 + d_5(\frac{T - T_r}{T_m - T_r})] \qquad (3)$$

Where p is the hydrostatic pressure, q is the effective stress, d1, d2, d3, d4 and d5 are material parameters.

Under high strain rate condition, the producing of plastic strain is a transient process, during this time the diffusion of heat is low, we can assume it to be an adiabatic process that the heat conduction is negligible. But the temperature effect, as a field variable, on material constitutive relation can't be ignored, heat increment result of plastic work per unit volume is:

$$dr^{p} = \eta\sigma d\varepsilon^{p} \tag{4}$$

Where η is the fraction of plastic work converted to heat, it is assumed a constant 95% here. By thermal governing equation, the differential of temperature is:

$$dT = dr^{p} / (\rho c^{p}) \tag{5}$$

Where, ρ is density and c^{p} is specific heat. Thermal expansion effect can't be ignore since the dramatically change of temperature in ASBs. Thermal strain is linear function of temperature rise:

$$\varepsilon^{T} = \alpha dT \tag{6}$$

Where α is coefficient of thermal expansion. In FEA region, material parameters of copper are obtained from paper of Li (2010)

MD simulation is based on EAM potential, basic idea of EAM is that total potential of an atom can be divided into two part parts, one is pair potential which represents interaction between two atoms and another is embedded potential. Total potential of EAM can be written:

$$E = \sum_{i} F_{\alpha}\left(\rho_{i}\right) + \frac{1}{2}\sum_{j \neq i} \phi_{\alpha\beta}\left(r_{ij}\right) \tag{7}$$

Where, F is the pair potential, and ϕ is the embedded potential (Finnis 1984).

For copper, fcc single crystal structure was used to establish the MD model, lattice constant of copper is 0.344nm. To save computational resource, only one layer of atoms on (0 0 1) of fcc crystal was involved in calculation, and periodic boundary condition was applied in through-thickness direction. We used NVE ensemble with velocity rescaling method to keep the temperature consistent with FEA temperature. The MD time step size was set as 0.001ps.

3 Results and discussion

3.1 Macro and micro analysis of initiation and propagation of ASBs

Temperature and stress distribution under shear loading velocity of 30m/s at different time are shown Fig. 2 and Fig.3. The initial stage was chosen at t=30 us and the total time of observing was 35us. We can see that temperatures in shear bands are obviously higher than that in any other region (Fig.2). Since our analysis is under the condition of adiabatic, temperature increasing is only related to the plastic work. It means that temperature field is a characterization for plastic deformation localization. Stresses in shear bands region are lower than that in the vicinity of ASBs, which means that stress collapse when the effective plastic deformation reaches a certain amount (seeing Fig.3).

There is a high-temperature localized region where maximal temperature reaches 418K at 30us as shown in Fig.2 (a), it means that shear localized region initialized before the forming of shear bands; Von-Mises stress contour at the same time is shown in Fig.3 (a), the stress collapse is not obvious, but the maximal stress reaches 460MPa.

At 40us, the maximal temperature reaches 436K with the evolution of shear localized region, and there is an obvious shear bands in the sample (Fig.2 (b)); In Fig.3 (b), there is a stress collapse region which has similar shape and size with high temperature region in Fig.2 (b). We can also observe that the stress concentration region has move to the end of ASBs.

By comparison between ASBs feature at 50usand 40us (seeing Fig.2 (c) and Fig.3 (c)), we can see that: as the propagation of ASBs, the width of it is almost the same; Variation of maximal temperature is small since the plastic strain value is limited; Maximal Von-Mises stress is almost changeless and the stress collapse results in the redistribution of stress concentration.

Fig.2 (d) and Fig.3 (d) show that: at 65us shear bands propagate through the sample and there is no stress concentration region which means that the sample has lost the loading capacity.

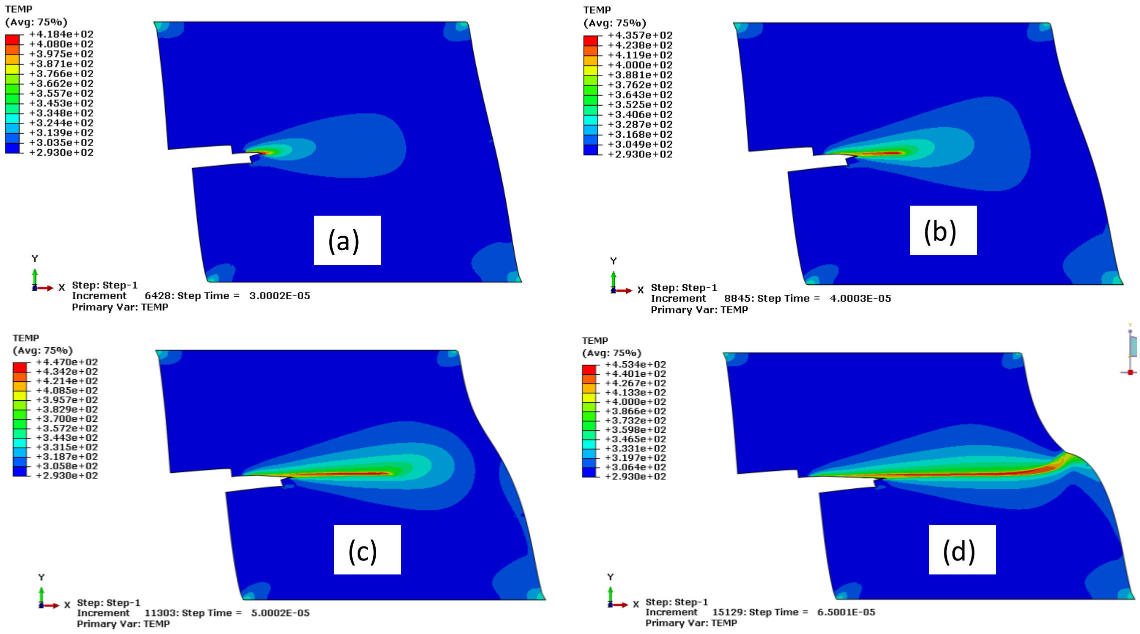

Fig.2 temperature contours for shear sample,
（a） t=30us （b） t=40us （c） t=50us （d） t=65us

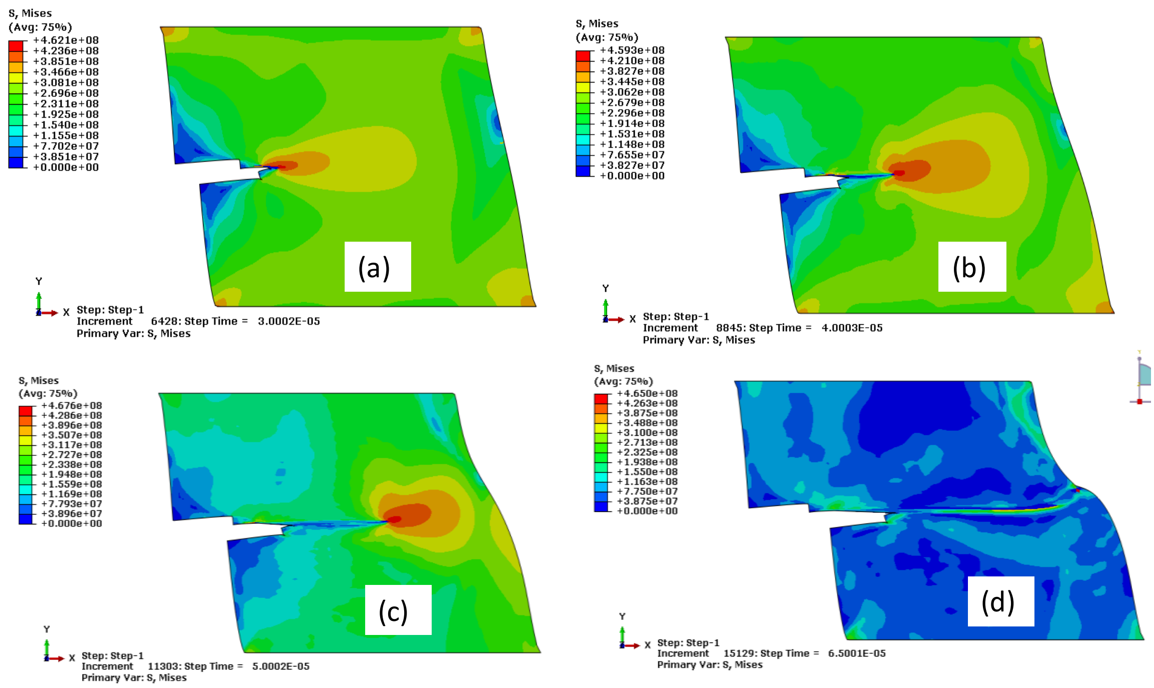

Fig.3 Von-Mises stress contours for shear sample,
（a）t=30us（b）t=40us（c）t=50us（d）t=65us

To get quantitative variation of stress and temperature on plastic strain, one element „Element397' in the shear band (as shown in Fig.4 (a)) was analyzed. Stress-strain curve and temperature-strain curve for „Element397' are given in Fig.4 (b). The Fig.4 (b) shows that both curves can be divided into three stages:(1) Linear elastic deformation stage. There is only uniform deformation in the element and the temperature was unchanged; (2) Plastic deformation stage. When the temperature is relatively low, the thermal softening effect is not obvious, and the strain hardening and strain-rate hardening effect dominate the stress change. With the increase of temperature, the rate of stress change slows down and stress saturates to value of 460MPa, this is due to the mutual effect of strain hardening, strain-rate hardening and thermal softening; (3) Damage stage. When the plastic strain reaches a value of 1.1, the stress drops down to zero quickly and the temperature increases rapidly to 500K. We can conclude that instable adiabatic shear failure occur in this element. The maximal temperature in the sample is 500K, which is far less than the melting point of the OFHC copper, so melt is not a mechanism of the forming of ASBs.

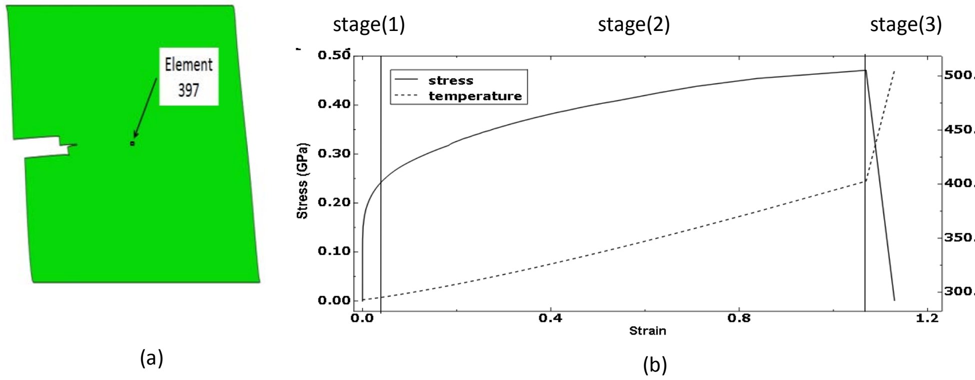

Fig.4 local element analysis, (a) position of #397 element. (b) stress-strain curve and temperature-strain curve.

At the initiation stage of ASBs, when t=30us, FEA results of temperature and displacement in the crack tip region were passed into MD model. By MD relaxation for 8ps, microstructure evolutions in vicinity of crack tip are depicted in Fig. 5. The Fig. 5(a) shows the micro structure of crack tip region after 2ps of MD relaxation, we can observe that secondary crack initial in orientation of 45 degree with the original crack orientation. At 4.5ps (Fig. 5(b)), more secondary cracks initial and some of them has propagate to MD boundary. At 6ps (Fig.5 (c)) micro voids initial in the sample and secondary has penetrated the whole MD region.

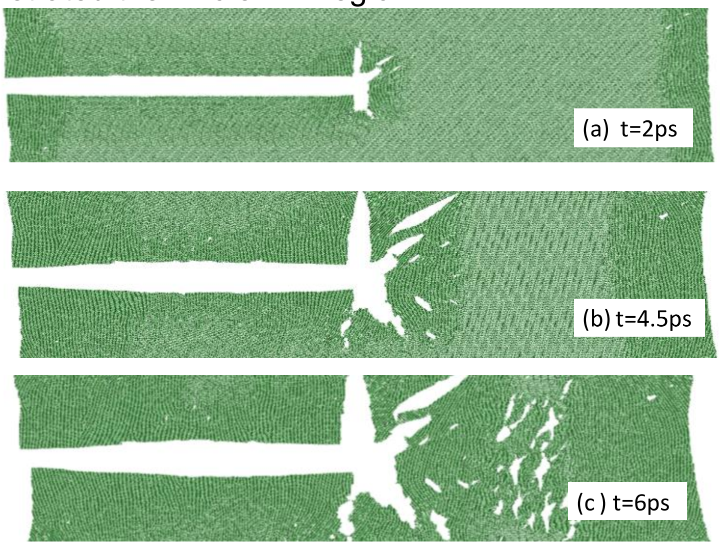

Fig.5 microstructure evolution in crack tip region at the initiation stage of ASBs, (a) t=2ps (b) t=4.5ps (c) t=6ps

3.2 Effect of shear loading rate on the initiation and propagation of ASBs

There are many factors, such as material property, load mode and rate that have effect on the ASBs, here we just analyze the effect of loading rate. Loading velocity V=20m/s, 30m/s, 40m/s, 50m/s were chosen, length history of ASBs are given in Fig.6. From the Fig.6, we found that less time is needed for the ASBs initiation as the increasing of loading rate. Meanwhile, penetration of the sample by ASBs also takes less time with the increasing of loading rate. It reflects that higher loading rate reduce the resistance of adiabatic shear.

History of propagation velocities are shown in Fig.7. All of these results have a trend in common that: the propagation velocities increase at first and then reach a peak value, after that the velocities drop rapidly. It can be observed that the loading rate has a big effect on the peak value of propagation velocity.

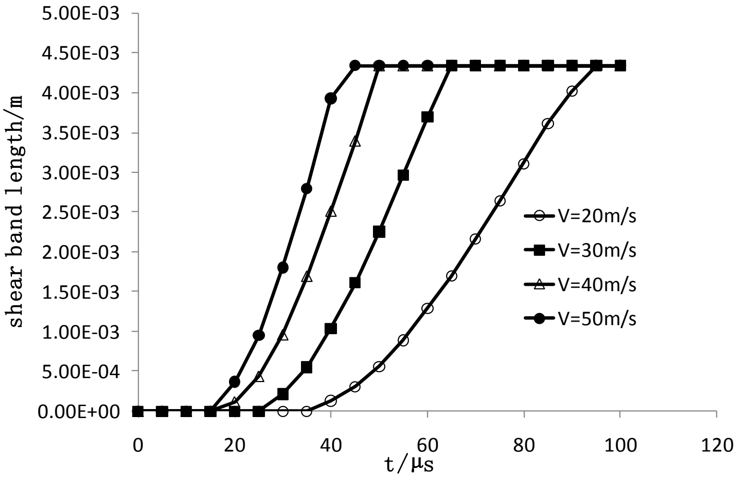

Fig.6 Length history of ASBs

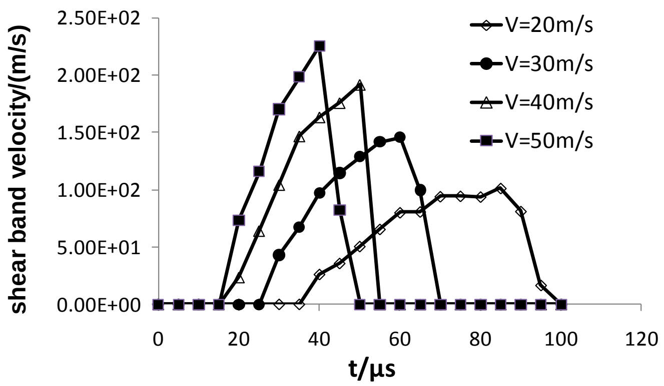

Fig.7 velocity history of the propagation of ASBs

It is widely accepted that criterion for ASBs is closely related to the temperature, so temperature is an important issue in studying ASBs. „Element397', as mentioned before, was used to study the temperature change in ASBs. Temperature history curves of „Element397' under different loading rate (Fig. 8) show similar trend, they increase slowly with time at first and then increase quickly to saturated values. The saturated values are also related to the loading rate, when the loading rate increase, the saturated values of temperature increase.

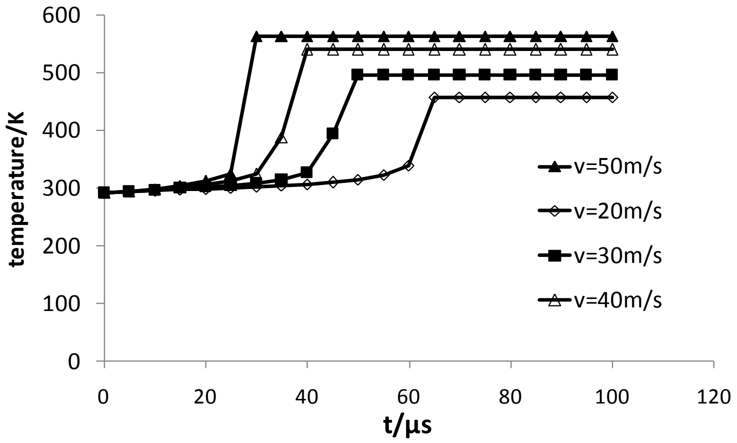

Fig.8 Temperature history in #397 element

4. Conclusions

The initiation and propagation of ASBs is a multiscale process which span macro-scale and micro-scale, a multiscale approach that coupling MD and FEA was propose to simulate and analyze the ASBs. Johnson-Cook constitutive model and damage model was used in FEA simulation. By FEA calculations, temperature field and stress field were obtained. During the propagation of ASBs, temperatures only show little change while the stresses collapse with the propagation of ASBs. By MD calculations in crack tip region it was found that at the initiation stage of ASBs, secondary cracks and voids initiation in the vicinity of original crack tip.

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