Magnesium Technology 2011
Edited by: Wim H. Sillekens, Sean R. Agnew, Neale R. Neelameggham, and Suveen N. Mathaudhu
TMS (The Minerals, Metals & Materials Society), 2011

A molecular dynamics study of fracture behavior in magnesium single crystal

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Keywords: molecular dynamics simulation, crack propagation; magnesium single crystal; temperature effects; strain rate

Abstract

The analysis of crack growth in magnesium crystals was performed using molecular dynamics simulation with Embedded Atom Method (EAM) potentials. Four specimens with increasing sizes were used to investigate the influences of material length scale on crack growth of magnesium single crystals. Furthermore, the effects of temperature, loading strain rate, and the size of the initial crack were also verified. The specimens were subjected to uniaxial tension strain up to the total strain level of 0.2 with a constant strain rate of $10^9 s^{-1}$ except in the studies of strain rate effects and the uniaxial stress strain curve was monitored. The simulation results show that the specimen size, loading strain rate, temperature, and the size of initial crack strongly influence the yield strength at which the twin nucleated and subsequently the crack grew. The initial slope of the uniaxial stress strain curve is independent of the loading strain rate and temperature. Moreover, high temperatures induce increased atomic mobility, and thereby atom reorganization, which, in turn, releases the stress at the crack tip

Introduction

The study of materials' fracture behavior has been the topic of intensive research in the physical and engineering sciences since last century. Numerous achievement has well established the continuum-based theoretical framework of fracture mechanics at the macro scale. Griffith first proposed a continuum fracture model for predicting the onset of crack growth in a brittle material based on energetic and thermodynamics considerations [1, 2] and the earlier work of Inglis [3]. After his seminal contribution, fracture mechanics theories were developed to account for the nonlinear behavior of materials such as plasticity and viscoplasticity at the crack tip [2].

Meanwhile, the fracture mechanism in nanocrystalline materials is not clearly understood. To reveal the mechanism of fracture at the nanoscale requires discerning the evolution process of the crack tip under the application of increased stress intensity, which is strongly affected by the local atomic structure, lattice orientation, interatomic potentials, and generation of defects (e.g., dislocations and twins). With the rapid development of computer technique as impetus, molecular dynamics (MD) has become an increasingly important tool for studying the fracture behavior at atomic scale. MD simulations predict the motion of atoms in an atomistic system through Newton's equations of motion. Combined with the initial and boundary conditions, these equations can be solved using numerical integration method to obtain the trajectories of atoms such as the position and velocity as a function of time.

During the past several decades, MD has been widely employed to investigate fracture problems. These studies include the fast brittle fracture in a material [4, 5, 6, 7], instability of dynamic fracture in three-dimensional fracture [8, 9], brittle-to-ductile transition (BDT) in crack growth [10, 11], stress-induced phase transformations and grain nucleation at crack tip [12], influences of grain boundary [13, 14], and large-scale MD simulation of three-dimensional fracture [15]. Moreover, Rafii-Tabar *et al.* [16] used MD simulations to study the effects of nanoscale inhomogeneities near the crack tip on the crack propagation in fcc metallic plates. Recently, Xu and Deng [17] performed MD simulations of ductile crack growth in an aluminum single crystal and provided insight to the stress field around the crack tip and its evolution during crack growth. They concluded that the ductile crack growth in aluminum single crystal was achieved via void nucleation, growth, and coalescence ahead of the crack tip. However, few studies have been published on the fracture behavior of magnesium.

In this study, we performed MD simulation of crack propagation in magnesium crystals using Embedded Atom Method (EAM) potential. The goal of the present work was to elucidate the influences of spec-

imen size, temperature, strain rate, and initial crack length on the fracture behavior of magnesium single crystals. The uniaxial stress strain responses were monitored during uniaxial tension. The simulation results will help provide a better understanding of magnesium's fracture behavior at the nanoscale.

Simulation Method

The computation method used in this study is Embedded Atom Method (EAM) potential developed by Sun *et al.* [18]. This form of EAM consists of two contributions to the total potential energy, E, of the entire system composed of N atoms. The functional form of the total embedded energy can be expressed as

$$E = \sum_i G_i \left(\sum_{j \neq i} \rho_j^a \left(r_{ij} \right) \right) + \frac{1}{2} \sum_{ij} U^{ij} \left(r_{ij} \right) \quad (1)$$

where G_i is the embedding energy as a function of the local electron density, ρ_j^a is the speherically averaged atomic electron density, U^{ij} is the pair potential, and r_{ij} is the distance between atom i and j. Many examples have demenstrated that EAM can be an accurate representation of inter-atomic forces in a metallic lattice. In molecular dynamics, the energy is employed to determine the forces acting on each atom. At each atom the dipole force tensor, β_{ij}, is given by

$$\beta_{km}^i = \frac{1}{\Omega^i} \sum_{j(\neq i)}^{N} f_k^i \left(r^{ij} \right) r_m^{ij} \quad (2)$$

where f_k is the force vector between atoms, r_m is the displacement vector between atoms i and j, N is the number of neareast neighbour atoms, and Ω^i is the atomic volume. If stress could be defined at an atom, then β_{ij} would be the stress tensor at that point. Since stress is defined at a continuum point, the stress tensor can be determined as a volume average over the block of material,

$$\sigma_{mk} = \frac{1}{N^*} \sum_{i}^{N^*} \beta_{mk}^i \quad (3)$$

in which the stress tensor is defined in terms of the total number of atoms, N^*, in the block of material.

Specimens for atomistic studies

The size effects on crack growth were studied using four specimens of increasing size as shown in Fig. 1.

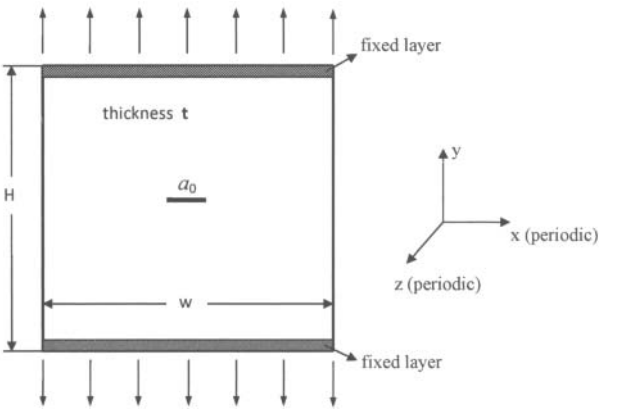

Figure 1: Model geometry of magnesium single crystal containing a center initial crack.

Table 1: Geometrical dimensions and the resulting number of atoms of the specimens of increasing size.

sp #	w (nm)	H (nm)	t (nm)	# of atoms
1	6.0	9.0	2.21	4,884
2	12.0	18.0	2.21	20,100
3	24.0	36.0	2.21	82,740
4	40.0	60.0	2.21	229,900

The sizes of the four specimens were generated by increasing the width and the height of the specimen but maintaining the thickness, t, as a constant. The ratio of height to width of in each of the specimens is kept constant as $H/w = 1.5$. A center crack introduced in each specimen by removing the atoms from the perfect crystals and maintaining the ratio of the initial crack length to the width of the specimen to $a_o/w = 0.1$. The resulting number of atoms varied from 4884 to 229,900. Table 1 presents the geometrical dimensions and the resulting number of atoms in the four specimens of increasing size. The edges of the specimens were aligned with the global coordinate system in which the x axis represents $[12\bar{1}0]$ direction, the y axis represents [0001] direction and the z axis represents $[10\bar{1}0]$ direction.

Simulation process

For both single crystal and bicrystal specimens, the top and bottom boundaries are free surfaces. About 1 nm deep atomic surface layers at the top and bottom boundaries were fixed for applying Mode I cyclic loading. For single crystal specimens, the periodic

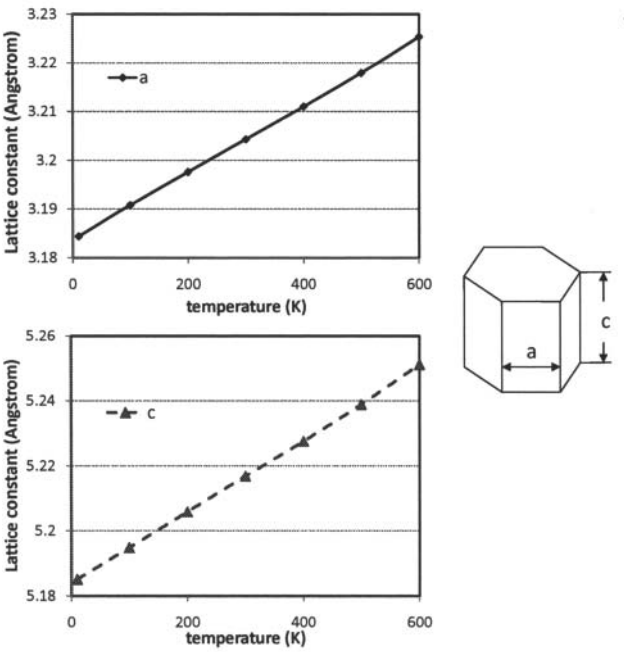

Figure 2: Variation of lattice constants of magnesium crystal with temperature.

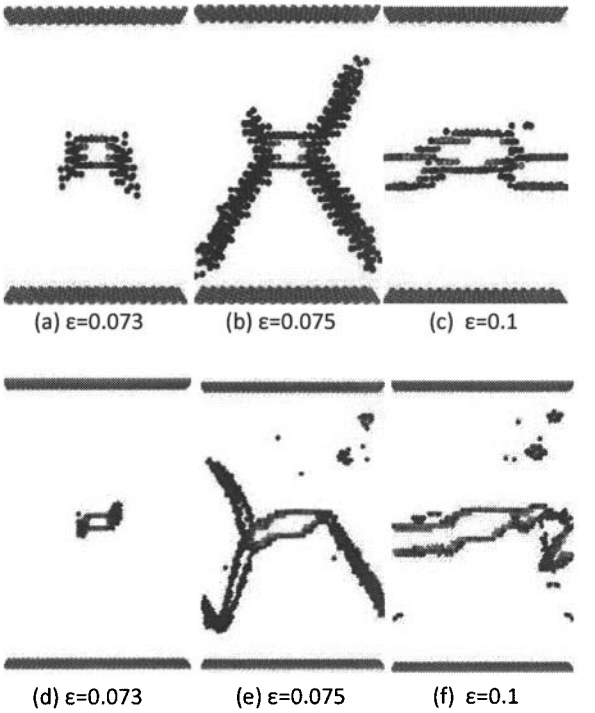

Figure 3: Crack growth and twin pattern of different specimen size at various applied strain: (a), (b), and (c) are the contour plot of the smallest size specimen-1 with 4884 atoms; (d), (e), and (f) are the contour plot of specimen-2 with 20,100 atoms.

boundary conditions were assigned in the $x-$ and $z-$ directions. In all simulations, the specimens were equilibrated at 100 K (except in the studies of the effects of temperature) by running 2000 timesteps before applying uniaxial tension loading. The uniaxial tension strain loading was applied along the y axis up to the total strain of $\epsilon_y = 20\%$. For the sake of eliminating the stress oscillation resulting from the sudden loading employed on the top and bottom boundary, the loading was applied such that the velocity was linearly distributed along the $y-$ direction from the bottom to the top. The velocities were maximum positive value and minimum negative value at the top and bottom boundary, respectively. The uniaxial tension loading was applied at a constant strain rate of $10^9 s^{-1}$ except in the studies of strain rate effects. All simulations were performed at a constant temperature of 100 K except in the studies of the effects of temperature.

Lattice constants

To study the temperature effects on fatigue crack propagation, we calculated the lattice constants of magnesium at various temperatures. In this calculation, we created a three dimensional model without defects. Periodic boundary conditions were assigned to all of three directions so that the thermal expansion of the model was isotropic. This model was firstly equilibrated at constant temperature and zero pressure. The temperature was controlled by rescaling the velocities of atoms while the pressure of the model was set to zero by using a Berendsen barostat. Finally, constant NPT integration was performed upon the group of atoms to update positions and velocities at each time step. P is pressure and T is temperature. This created a system trajectory consistent with the isothermal-isobaric ensemble. The variation of lattice constants c and a are plotted in Figure 2.

Simulation results and discussions

This section presents the MD simulation results for verifying the effects of the specimen size, temperature, strain rate, and grain boundary on the crack growth in magnesium crystals. The centrosymmetry parameter defined by Kelchner *et al.* [19] was used to highlight the defects including void surface and twin.

The expression of this parameter is given by

$$P = \sum_i |R_i + R_{i+6}|^2 \quad (4)$$

where R_i and R_{i+6} are the vectors or bonds corresponding to the six pairs out of twelve nearest neighbors in the lattice. The six pairs are chosen to minimize P. The P values for the atoms in fcc and hcp structures, dislocations, twinning boundaries and crack surfaces are all different so that extensive information about crack growth and many defect behaviors can be obtained.

Size effects

The material length scale has apparent influences on the strength, toughness, ductility, and the stress strain response of materials [20, 21, 22, 23]. In this study, the investigation of size effects on the crack growth was performed using the four specimens of increasing size as specified in Fig. 1 and Table 1. The simulation results of different specimen sizes are shown in Fig. 3 and 4. The uniaxial stress strain curves of different specimen sizes obtained from MD simulation are plotted in Fig. 5. One common feature of all specimen sizes is that the twin nucleated at the crack tips due to the stress concentration just after the yield strength is reached as shown in Fig. 3(a), Fig. 3(d), Fig. 4(g), and Fig. 4(j). This means that the yield strength corresponds to the nucleation of twin bands. The stress resistance dropped down abruptly after yielding. As the external loading continues increasing, more twin bands are initiated and grow from the crack tips. Meanwhile, the crack starts growing just after the yield is reached. The paths of crack extension are significantly influenced by the twin bands being nucleated and grown from the crack tips. Finally, the stress resistance decreased to almost zero when the crack reached the specimen edges.

From Fig. 3, 4, and 5, we can observe the significant size effects. Different specimen sizes demonstrate different twin patterns and crack growth paths. At larger specimen sizes as shown in Fig. 4, the right crack propagates along the twin band with mixed Mode I+Mode II. It is observed that the crack propagated rapidly along the twin band with a manner of brittle fracture. The initial yield strength decreases with increasing specimen size. At the smallest specimen size, the yield strength is about 11.2 GPa while it decreased to about 6.3 GPa at the largest specimen size. On the other hand, the size effect de-

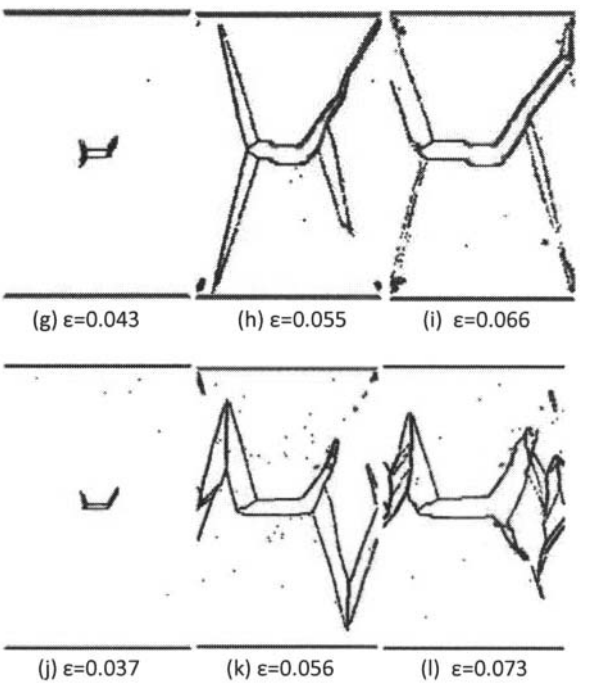

Figure 4: Crack growth and twin pattern of different specimen size at various applied strain: (g), (h), and (i) are the contour plot of specimen-3 with 82,740 atoms; and (j), (k), and (l) are the contour plot of specimen-4 with 229,900 atoms.

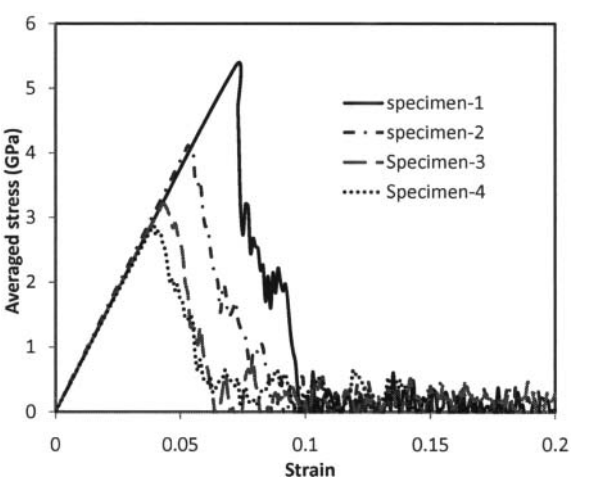

Figure 5: Influences of specimen size on the averaged stress strain response of magnesium single crystal specimen containing a center initial crack.

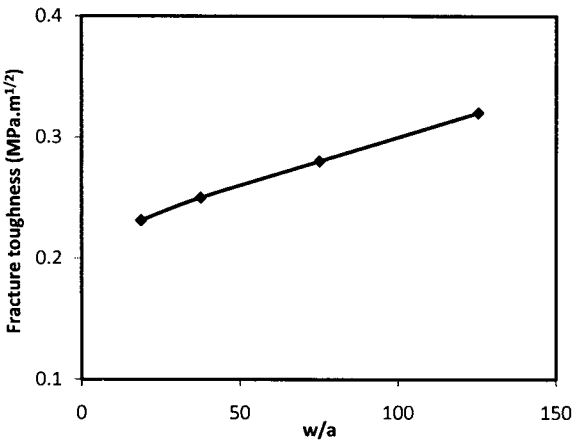

Figure 6: Variation of fracture toughness with the normalized specimen size.

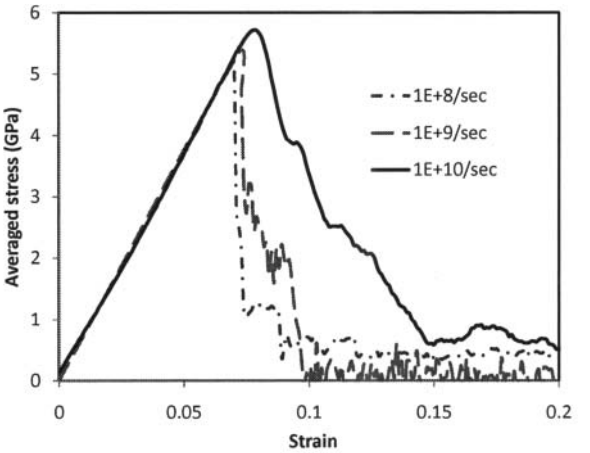

Figure 7: Effects of strain rate on the averaged stress strain response of magnesium single crystal specimen containing a center initial crack.

creases with increasing specimen size. The initial slope of the uniaxial stress strain curve of the smallest specimen is little lower than those of larger specimens. As the material length increasing, the initial slopes of the uniaxial stress strain curves are independent of the specimen size. Since the crack propagated rapidly and unstably after the initial yielding strength is reached, the values of the stress intensity factors at the yielding strength, K_{IC}, of different specimen sizes are nanoscale fracture toughness and can be expressed as

$$K_{IC} = Y\sigma\sqrt{\pi a} \tag{5}$$

where σ is the volume averaged stress in the $y-$ direction; a is the initial crack length; the value of geometrical factor Y is about 1.016. For simplicity, Y is assumed to be 1. Fig. 6 presents the variation of nanoscale fracture toughness with the normalized specimen size, the ratio of the length w of the specimens to the lattice constant a of magnesium. We can observe that the fracture toughnesses at nanoscale increase with increasing specimen size even though the values of peak stress points decrease with increasing specimen size. This effect results from the initial crack length increases with increasing specimen size at the same time.

Strain rate effects

For the sake of reducing computational cost, the investigation of strain rate effects was performed on the smallest specimen. Fig. 7 shows the stress-strain responses obtained from three strain rate levels, namely, 10^8, 10^9, and 10^{10}s^{-1}. One apparent finding is that the initial slopes of the uniaxial stress strain curves were independent of the strain rate. After the yielding strength is reached, the stress response decreases rapidly. The yield strength increases with increasing strain rates. On the other hand, the yield strength is getting insensitive to the strain rates with decreasing strain rate. The results are qualitatively similar to those obtained from Potirniche *et al.*'s studying on the strain rate effects on void growth and coalescence [23].

Temperature effects

In the previous studies, the simulations were carried out at a constant temperature of 100 K. It is well known that temperature has significant influences on the material properties. To study the effects of temperatures, we constructed the atomistic models with different lattice constants obtained from various temperatures, namely, 10 K, 100 K, 300 K, and 500 K. The lattice constants of various temperatures are shown in Fig. 2. The size of atomistic models of different temperatures is the same as $w(12nm) \times H(18nm) \times t(2.21nm)$. Fig. 8 shows the uniaxial stress strain curves of various temperatures. In general, the stress resistance dropped down rapidly after the yield strength is reached at all temperatures. It is seen that the initial slopes of the uniaxial stress strain curves are independent of temperature. The yield strength decrease with increasing temperature due to the degradation of materials at higher temperature. This phenomenon implies that the critical stress of twin nucleation decreases with increasing

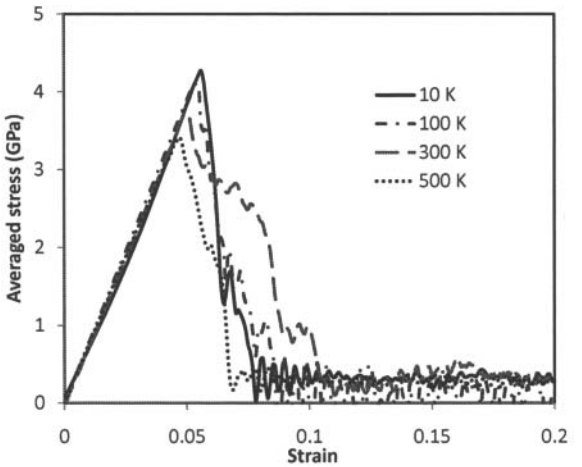

Figure 8: Temperature effects on the averaged stress strain response of magnesium single crystal specimen containing a center initial crack.

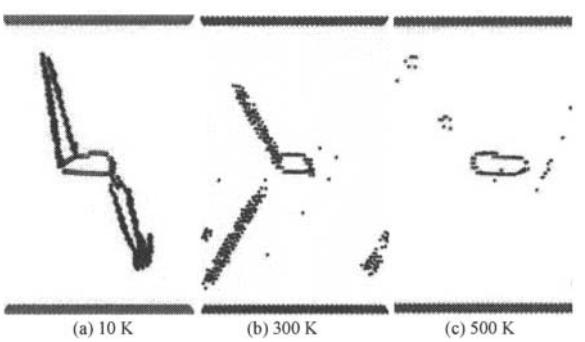

Figure 9: Simulation of crack growth in magnesium single crystal at various temperatures when the applied tension strain is $\epsilon_y = 0.06$.

temperature. Fig. 9 shows the contour plot of crack growth at different temperatures. The twinning at the crack tip becomes weak with increasing temperature and eventually disappears at 500 K. At high temperature 500 K, the stress concentration at the crack tip was significantly alleviated by the reorganization of atoms due to the high mobility of atoms at high temperature. This effect causes the twinning vanishing and the crack tip being blunted. This phenomenon is similar to the observation of Latapie and Farkas [12]. We can deduce that a brittle-to-ductile fracture behavior is induced by increasing temperature.

Conclusions

We have performed the MD simulations of crack growth in magnesium crystals using EAM potential at nanoscale. Single crystal specimens were used to study the influences of specimen size, strain rate, temperature, and initial crack length. The investigation of the effects of grain boundary was carried out using three bicrystal models with different misorientations. According to the simulation results, the following conclusions were obtained:

1. The significant size effects were clearly demonstrated by uniaxial averaged stress strain responses. The yield strength decreases with increasing specimen size. The initial slope of the average stress strain curve is independent of the specimen size except the smallest specimen size. Meanwhile, it is also found out that the size effects decrease with increasing specimen size.

2. Furthermore, the yield strength decreases with increasing strain rate, and temperature. On the other hand, the initial slopes of average stress strain curves are independent of strain rate and temperature. The twinning becomes weak and the material becomes ductile at high temperature so that the resistance of crack growth increase with increasing temperature. This effect results from the stress at the crack tip being released by the reorganization of atoms due to the high mobility of atoms at high temperature.

3. In all loading conditions and specimen sizes, the decrease of averaged stress strain response is mainly due to the nucleation of twinning at the crack tip followed by the crack starting propagation.

Acknowledgement

The authors acknowledged the Center for Advanced Vehicular Systems at Mississippi State University and the Department of Energy for supporting this research.

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