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Editor's Choice

Effects of quenching rate on crack propagation in NiAl alloy using molecular dynamics

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ABSTRACT

The crack growth and propagation of pre-cracked NiAl alloy prepared at different quenching rates under mode I loading conditions were investigated using molecular dynamics (MD) simulation based on the many-body embedded atom method (EAM) potential. The quench rate effects were evaluated in terms of atomic trajectories, common neighbor analysis (CNA), radical distribution function (RDF) and glass transition. The simulation results clearly show that as the quenching rate increases ten times from 0.5 K/ps to 50 K/ps, the volume after quenching will increase by approximately 1%. The amorphous structure and crystalline structure exhibit two distinct types of fracture behavior between quenching rates of 0.25 –50 K/ps. In the amorphous state, the critical stress increases with decreasing quenching rate. Moreover, two shear bands and the shear transformation zones (STZ) extend along a direction of about 45° with respect to the horizontal direction away from the crack tip.

1. Introduction

Metallic glasses (MGs) have emerged as a prospective structural material in recent years. They possess excellent properties, such as high strength, high elastic limit, high ductility and superior corrosion resistance [1–7]. Therefore, they have potential for applications in the fields of micromachine, microelectromechanical, and nanoelectromechanical systems [8–10]. Even though metallic glass has many beneficial applications, instantaneous brittle failure, however, leads to a fatal shortcoming. This phenomenon may be different at the nanoscale. Thus, it is important to understand the material deformation under applied strain at the nanoscale.

In materials science, crack growth or propagation in polycrystalline metal maybe either transgranular or intergranular, whereas that in single crystal metal may be either slip or dislocation, and in amorphous metal, it maybe shear bands. Generally speaking, the glass-forming ability of MGs depends on the quenching rate; the larger the quenching rate, the higher the glass-forming ability (GFA) [11]. Therefore, it is an interesting task to determine the relationship between crack propagation and quenching rate. Moreover, the growth of shear bands is particularly important due to the fact that they are key features related to controlling plasticity and failure in MGs [12–14].

Molecular dynamics (MD) simulations can provide the fundamental mechanism of the mechanical properties and material fracture behavior on the micro/nano scale. It is a powerful tool for studying material behavior and provides detailed deformation information at the atomic level. An atomic simulation avoids experimental noise and turbulence problems and can be used to analyze atomic trajectories and both thermodynamic and mechanical properties. Numerous classical simulation and computational studies have been conducted on material properties and failure modes of MGs at the atomic level, including the effect of temperature on the structure [15], size-dependent brittle-to-ductile transition [16–20], fractures via shear band cavitation or pores [21,22], the effect of quenching and component and structure concentrations on mechanical behavior [23–27]. However, simulations on shear band-to-crack transitions with different quenching rates are still lacking in the literature. Further important information on shear band-to-crack transition in MGs can be obtained by the direct calculation of the variations in the internal stress in shear bands. Due to the fact that a shear band has a spatial scale of nanometers and a temporal scale of nanoseconds or less, the onset of a fracture is extremely difficult to describe in experiments. For this reason, MD simulation was selected in this study.

To investigate the relationship between crack propagation and the quenching rate of MGs, MD simulation under mode I (opening mode) loading conditions with embedded atom method (EAM) potentials was selected as the simulation system. The effects of quenching rate on the deformation and mechanical properties of

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$Ni_{50}Al_{50}$ alloy from the crystalline (B2 structure) to the amorphous state with a crack and an infinite length in the y direction were examined. Among NiAl structures, B2 (CsCl-type, Pm-3m) is the most stable one both at ambient. Moreover, the phase diagram shows only one-phase B2 structure of Ni50Al50 binary system between the room temperature and melting point [28,29]. Therefore, B2 was treated as a unique phase. This work contributes to the understanding of nanomechanical properties, deformation, crack propagation and growth around the crack tip for a pre-cracked NiAl alloy under tensile stress for nanosystem applications. The results are quite different from those of previous cases and are discussed in terms of atomic trajectories, atomic strain, stress fields, slip vectors, critical strength, and radial distribution function (RDF).

2. Methodology

The MD simulations were carried out using the LAMMPS Package (Large-scale Atomic/Molecular Massively Parallel Simulator, http://lammps.sandia.gov) [30]. A B2 crystal structure containing the same Ni and Al atoms was used. The size of the initial model was $120a \times 120a \times 12a$ ($34.68 \times 34.68 \times 3.47$ nm), where a (= 0.289 nm) is the lattice constant of NiAl. An edge crack was inserted on the left side of the model. The length of the initial crack was equal to $10a$ (2.89 nm), and its width was $5a$ (1.45 nm). A Cartesian coordinate system was used in the proposed system. The amorphous alloy model was prepared by simulating melting and quenching. The most at atom velocities were adjusted in order to maintain them in an isothermal state with a specific temperature, obeying Newton's second law. The model was initially relaxed under periodic boundary conditions at 293 K for 200 ps within an NPT (constant pressure and constant temperature) ensemble. The model was then heated up to 2500 K and kept for 300 ps, allowing the solid to melt using the conjugated gradient method [31]. After that, the model was kept at 2500 K for 40 ps and quenched to 50 K with a variable quenching rate ranging from 0.25 K/ps to 50 K/ps, as shown in Fig. 1. At slow cooling rates, dendrites have more enough time to grow before they begin to touch neighboring dendrites. Therefore, a more large grain size is formed in this way, as shown in Fig. 1(d). At fast cooling rates, a lot of dendrites grow quickly and are restricted by other dendrites. Consequently, a more fine grain size is formed in this way, as shown in Fig. 1(b) and (c). If the cooling rate is high enough, the atoms do not have enough time to rearrange themselves for crystal. The liquid state maintains right up to the room temperature and then solidifies as metallic glass, as shown in Fig. 1(d). During the deformation process, the periodic boundary condition was applied in the y and z directions, and the model was uniaxially loaded by rescaling the simulation box with a strain rate of 0.4 ns^{-1} at 50 K. The many-body potential embedded atom method (EAM) was adopted to describe the Ni–Ni, Al–Al and Al–Ni interactions. The total energy E_i of every atom i satisfies [32]:

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

where r_{ij} is the distance between atoms i and j; $\phi_{\alpha\beta}$ is a pair of potential interaction parameters; F is the embedding energy, which is a function of atomic electron density ρ and α and β are the element type parameters of atom i and atom j. The time integration step of 1 fs and the lists of neighbor atoms were calculated every 10 time steps with a cut-off radius of 0.55 nm. In order to analyze the atomic structure of the MGs, the common neighbor analysis (CNA) [33] and RDF [34] methods were applied in the simulation. The RDF describes how the atomic density varies as a function of the distance away from one particular atom, which can often be used to identify the crystal order. The RDF function is defined as

$$g(r) = \frac{N(r,\Delta r)}{\frac{1}{2}N\rho V(r,\Delta r)} \quad (2)$$

where N is the total number of atoms; V is the system volume; ρ is the number density ($\rho = N/V$); $N(r, \Delta r)$ is the number of atoms found in a spherical shell of radius r and thickness Δr, with the shell centered on another atom, and $V(r, \Delta r)$ is the volume of the spherical shell. The analysis of the defects within the microstructure was conducted using CNA. The cut-offs for each interatomic pair were chosen between the first and second nearest neighbor shell around each atom.

3. Results and discussion

3.1. Formation and structural properties of NiAl alloy

In order to explore the structural characteristics of the initial undeformed state of amorphous alloys, glass transition and pair correlations are discussed in this section. Fig. 2 shows the volume changes in the simulated NiAl alloy as a function of temperature during the cooling process at three different quenching rates, 50, 5, and 0.5 K/ps, respectively. Fig. 2 illustrates the glass transition temperature dependence on the cooling rate. During the cooling process, the volume–temperature curve with a quenching rate of 50 K/ps shows a slope change at about 700 ± 50 K, which indicates that glass transition occurs at this temperature. However, with increasing quenching rates, the glass transition temperature (T_g) with one turning point transforms into freezing temperature (T_f) with two turning points, and the slope of the curve changes sharply over a narrow temperature range between two turning points, which indicates the amorphous solid transformed into a crystalline solid between the T_g and T_f. In the literature, thermodynamic transitions are classified as being either first- or second-order. The system experiences an abrupt volume change and a transfer of heat in the first-order transition. However, the system experiences a gradual volume change, and there was no transfer of heat in the second-order transition [35]. The glass transition is similar in appearance to a second-order phase transition, but it is not a true

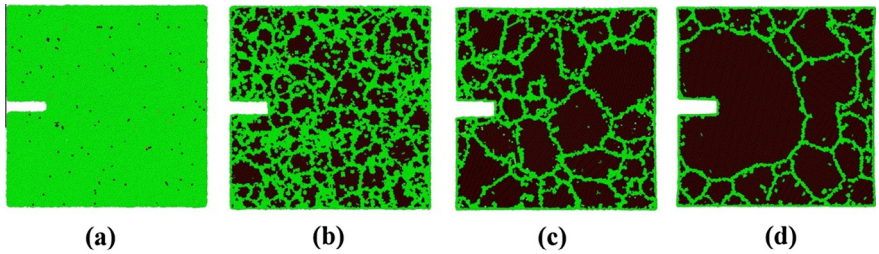

Fig. 1. CAN distributions with different quenching rates. The green atoms represent the amorphous structure, and the brown atoms represent the B2 structure. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)