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Effect of nitrogen content on the crack growth behavior in the Fe-N alloy at high temperatures via molecular dynamics simulations

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ABSTRACT

In this work, the influence of nitrogen content on the crack propagation behavior in Iron-Nitrogen (Fe-N) nanocrystalline was studied at high temperatures using molecular dynamics (MD). The semi-empirical Modified Embedded Atom Method (MEAM) potential function was utilized to model the interatomic interactions. The results revealed that at higher temperature of 900 K and 1100 K, more slip systems are activated resulting in the crack tip blunting ahead of crack tip and void nucleation and growth. Moreover, the results showed that the deformation mechanism and fracture behavior are significantly altered owing to the initial nitrogen concentration. The simulated results indicated the slow crack propagation at low nitrogen content of 0.1 wt.%. Detailed analysis confirmed that nitrogen concentration has a significant effect on the crack propagation. At high nitrogen content (0.51 wt.%), the crack growth increased by changing the crack propagation path.

1. Introduction

Fatigue resistance and mechanical properties of materials are of imperative significance in industries. Thermochemical processing is extensively used to enhance superficial mechanical properties such as residual stresses and hardness [1]. The nitriding process is very efficient amongst the thermochemical heat treatments, in spite of its extreme cost. Nitriding is frequently utilized in the manufacturing of automotive components, turbine generation systems, bearings and aircraft [2]. Due to the diffusion of nitrogen, precipitation of nanometric nitrides at grain boundaries occurs which leads to generation of compressive residual stresses in the near surface layers and an increase of hardness [3]. One of the major aims in nitrided materials is to predict the failure. Failure analysis is directly related to the stress concentration around the crack tip. Therefore, the fatigue resistance of materials subject to applied stress is controlled by atomistic mechanisms of crack growth [4,5].

Crack initiation, often modeled by strain (or stress)-life, has traditionally been considered to be a different phenomenon from crack propagation. However, some recent models of fatigue crack growth have been based on the assumption that each crack growth increment is physically similar to the initiation process. That is, the individual crack growth increments are successive initiations of the crack locally at the crack tip [6]. Noroozi et al. [7], and Hurley et al. [8] developed approaches to represent fatigue crack propagation using local fatigue models based on strain parameters. More recently, fatigue evaluation of notched details based on unified local probabilistic approaches was also proposed by Huffman [6] considering the Walker-like strain-life relation in conjunction with the probabilistic model proposed by Castillo and Fernández-Canteli [9]. Numerical simulation methods based on theoretical models showed its power in predicting phenomenon and obtaining quantitative results by evaluating atomistic arrangement and stress field in the vicinity of crack tip [10,11]. For instance, simulation of system containing one billion atoms has been realized by Buehler et al. [12]. Compared with other simulation methods as finite element analysis, Molecular Dynamics (MD) simulations are able to provide insights of various types of defects at nanoscale. MD is based on the assumption of treating atoms as classical particles, the motion of which obey Newton's Law. MD simulations have wide application fields, from chemistry, physics, and material science to biochemistry, biophysics and fluid dynamics [13]. Numerous studies have been conducted on the crack growth and crack tip dislocations in divers metals using MD simulations [14–17]. Since it is difficult to investigate by experiments further details of the phenomena, such as where and in what directions do cracks initiate or propagate, researchers tend to employ simulation methods such as finite element analysis [18] and MD simulations [19]. Conventional finite element method (FEM) can be capable of dealing with macro-scale material rather than micro-scale one such as at atomic-level. Compared with finite element analysis, MD simulations

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Table 1
2NN-MEAM potential parameters for pure Fe and N [33].

Element	E_c (eV)	α	A	$\beta^{(0)}$	$\beta^{(1)}$	$\beta^{(2)}$	$\beta^{(3)}$	$t^{(0)}$	$t^{(1)}$	$t^{(2)}$	$t^{(3)}$	$C_{\min}$	$C_{\max}$	ρ_0
Fe	4.29	5.07	0.56	4.15	1.00	1.00	1.00	1.00	2.60	1.80	-7.20	0.36	2.80	1.00
N	4.88	5.96	1.80	2.75	4.00	4.00	4.00	1.00	0.05	1.00	0.00	2.00	2.80	1.00

Table 2
2NN-MEAM potential parameters and fitting procedure for Fe–N alloy system [33].

Parameter	Selected value	Fitting procedure
E_c	$0.5E_c^{Fe} + 0.5E_c^{N} + 0.7$	Fitting dilute heat of solution of nitrogen in bcc Fe and heat of formation of Fe4N
r_e	2.09	Fitting lattice parameter of Fe4N
B	2.195	Fitting migration energy of a nitrogen atom in bcc Fe
d	$0.5d^{Fe} + 0.5d^{N}$	Assumption
$C_{\min}(Fe-N-Fe)$	0.16	For generally better agreement
$C_{\min}(N-Fe-N)$	0.16	Minimizing stability of unanticipated intermediate phases
$C_{\min}(Fe-Fe-N)$	0.16	Fitting vacancy–N binding energy in bcc Fe
$C_{\min}(Fe-N-N)$	$[0.5(C_{\min}^{Fe})^{1/2} + 0.5(C_{\min}^{N})^{1/2}]^2$	Assumption
$C_{\max}(Fe-N-Fe)$	1.44	For generally better agreement
$C_{\max}(N-Fe-N)$	2.80	Assumption
$C_{\max}(Fe-Fe-N)$	2.80	Assumption
$C_{\max}(Fe-N-N)$	2.80	Assumption
ρ_0	$\rho_0^{N}/\rho_0^{Fe} = 18$	For generally better agreement

are able to provide insights of various types of defects to nano-scale [20]. Therefore, MD method plays a significant role in capturing the general features of crack initiation and propagation at atomistic-level in alloys by associating macro-sale with micro-scale to reproduce macro-properties of a material [21]. With the rapid development in computer science technology, MD method be entitled to more consideration and is more widely used to analyze crack propagation mechanisms [22]. Therefore, MD can be a powerful tool for probing mechanical behaviors at atomic scale in the crack front.

Krull and Yuan [23] explored the crack evolution in the single-crystal aluminum and analyzed void nucleation by the stress concentrations in the vicinity of crack. Guo et al. [24] concluded that the stress concentration has a significant role in the phase transformation at the crack tip by MD simulation. Also, Xu and Deng [25] investigated void nucleation and growth mechanism at nanoscale in a single crystal aluminum. However, relatively less attention has been drawn on the Fe-N alloy systems due to the complexity of crystal structure. Zhang et al. [26] simulated the mechanisms of crack propagation in nanoscale single crystal, bicrystal and tricrystal nickels based on MD simulations. They indicated that the grain boundary has a key role in the crack initiation and increasing the velocity of propagation. An in-depth survey of the literature brought forth only one related study in MD simulation of crack in alloys [27]. In this study, the crack propagation in single crystal Ti-Al alloy is modeled by employing the embedded-atom method (EAM) interaction potential considering the influences of angle between a microcrack and loading direction.

Fracture behavior of nitrided iron based materials is strongly dependent on the nitrogen concentration, and temperature. The progress in system microstructure in the vicinity of crack tip may lead to the variation in the stress field and influence the fracture properties of nitride materials. As far as the authors know, there is no report on the MD simulation of crack in nitrided iron based alloys.

In order to illuminate the variation in the stress field in the vicinity of crack tip and fracture mechanisms, it is necessary to investigate

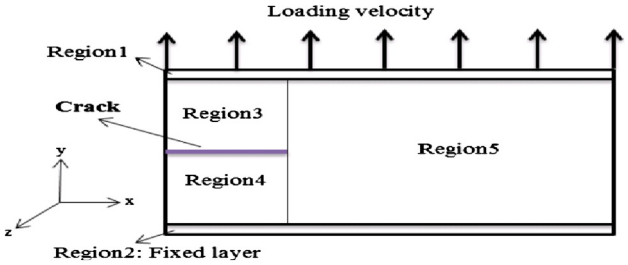

Fig. 1. The schematic diagram of different regions for crack propagation simulation in a single crystal, with an edge crack at the left side of the model.

nanoscale fracture behavior of Fe-N alloy system. The aim of this study is to illustrate the crack growth and failure process for a pre-cracked Fe-N crystal using MD simulation. The fundamental step in MD simulations is to select the suitable interatomic potential function for modeling the physical system. Hence, MD simulations carried out by applying Modified Embedded Atom Potential Function (MEAM) for Fe-N alloy. The MEAM potential has been applied for Fe-N nanocrystalline to investigate the diffusion process with and without strain conditions in the previous studies of authors [28,29]. In this study, the crack behavior illustrated through the evolution of system microstructure around the crack tip at different temperatures and nitrogen concentration.

2. Atomistic model and method

2.1. Modified embedded atom potential function

We examine the mechanism of crack growth in Iron-Nitrogen system through MD simulations. All atomistic simulations are performed with LAMMPS open source code [30] with MEAM potential to describe Fe-N systems. A flexible semi-empirical approach corresponds to interaction potentials among inclusive types of elements and their alloys by means of a common mathematical formalism. The MEAM interatomic potential function suggested by Baskes et al. [31] was the first semi-empirical atomic potential using a single formalism for different materials. The MEAM is an extension of EAM [32] to include e angular forces. The EAM is capable of reproducing physical properties of numerous metals and impurities.

The total energy E of a system of atoms in the MEAM is specified as the sum of the atomic energies:

$$E = \sum_i E_i \tag{1}$$

The energy of atom i involves the embedding energy and the pair potential terms:

$$E_i = \sum_i \left[F_i(\overline{\rho}_i) + \frac{1}{2} \sum_{i \neq j} \phi_{ij}(r_{ij}) \right] \tag{2}$$

where F_i is the embedding energy function for an atom i embedded in a background electron density $\overline{\rho}_i$ and $\phi_{ij}(r_{ij})$ is the pair potential interaction between atoms i and j separated by a distance r_{ij}.

The embedding energy $F_i(\overline{\rho}_i)$ represents the energy cost to insert atom i at a site where the background electron density is $\overline{\rho}_i$. The embedding energy is given in the form:

$$F_i(\overline{\rho}_i) = A_i E_i^0 \overline{\rho}_i \ln(\overline{\rho}_i) \tag{3}$$