



Molecular dynamics study of strain-induced diffusivity of nitrogen in pure iron nanocrystalline



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HIGHLIGHTS

- Mean square displacement was used to calculate coefficients of nitrogen diffusion in pure iron under strain conditions.
- Molecular dynamics shows that nitrogen diffusion is affected by the compression and tensile strain applied to the iron–nitrogen single crystal.
- Higher diffusion coefficients of nitrogen were obtained along [0001] crystal direction under compression.
- Diffusion is higher under compressive strain than tensile strain.

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ABSTRACT

In the present study, the self-diffusion process of nitrogen in pure iron nanocrystalline under strain conditions has been investigated by Molecular Dynamics (MD). The interactions between particles are modeled using Modified Embedded Atom Method (MEAM). Mean Square Displacement (MSD) of nitrogen in iron structure under strain is calculated. Strain is applied along [1120] and [0001] directions in both tensile and compression conditions. The activation energy and pre-exponential diffusion factor for nitrogen diffusion is comparatively high along [0001] direction of compressed structure of iron. The strain-induced diffusion coefficient at 973 K under the compression rate of 0.001 Å/ps along [0001] direction is about $6.72\text{E}-14\text{ m}^2/\text{s}$. The estimated activation energy of nitrogen under compression along [0001] direction is equal to 12.39 kcal/mol. The higher activation energy might be due to the fact that the system transforms into a more dense state when compressive stress is applied.

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1. Introduction

Surface hardening techniques are of importance for all practical applications where a hard surface is needed to resist wear, along with a tough substrate to resist the impact that occurs during operation. The advantages of nitriding applied to steel are nowadays widely recognized. During nitriding, the chemical composition of the surface layer is modified by the absorption and diffusion of nitrogen atoms. Numerous papers have been published concerning the gaseous nitriding of pure iron in lab scale reactors [1].

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Nitriding of iron-based alloys is broadly practiced in industries to enhance fatigue, wear, and anticorrosion properties of engineering components [2–4]. The nitriding alloys used for these applications contain many alloying elements. Therefore, it is difficult to understand the nitriding behavior of the alloys caused by a particular alloying element. In this regard, a sequential study of nitriding of pure iron, binary alloys etc., could be useful. Information about nitriding of pure iron is provided in detail in Refs. [1,5–7]. A systematic understanding of the nitriding behavior of iron based alloys has evolved over many years due to research by various authors for example, see Ref. [8] for nitriding of Fe–Ti alloys, Ref. [9] for nitriding of Fe–Al alloys, Ref. [10] for nitriding of Fe–V alloys, Ref. [11] for nitriding of Fe–Cr alloys.

Previous experiments and theoretical approaches has already faced the problems and the importance of stress effects revealed some aspects and their possible handling in solid state reactions [12–18]. For instance, the recent experiments of Schmitz et al. [19] pointed out that the intermixing rate could strongly be affected by stress, but surprisingly the parabolic growth rate is preserved. This is explained by the switching between the Darken and Nernst–Planck regimes forced by the diffusion-induced stress.

According to Boltzmann's transformation, a plane with constant concentration shifts proportionally with the square root of time [20] or in other words the solution of Fick's second equation as it was discussed previously results in the parabolic shift of planes with constant: or, where denotes the position of the monitored plane. Thus theoretical approach is suitable to investigate how the stress effects influence the diffusion kinetics.

Few researchers have studied the effect of stress on the displacement of nitrogen in iron alloys both experimentally [21] and analytically [22,23]. Moskaliuviene and Galdikas [22] explained the nitrogen distribution in plasma nitrided austenitic stainless steel at moderate temperatures is by non-Fickian diffusion model. The diffusion coefficient $D = 1.68 \times 10^{-12} \text{ cm}^2 \text{ s}^{-1}$ at nitriding temperature 380°C was theoretically found from fitting. In another study [23], they investigated the nitrogen transport mechanism in austenitic stainless steel during plasma nitriding at moderate temperatures by stress induced diffusion model. It was found that nitrogen diffusion coefficient varies with nitrogen concentration according to well-known Einstein–Smoluchowski relation $D(C_N) = f(1/C_N)$. It was shown that, with the increase of nitriding time, the compositionally-induced stresses and thickness of stressed steel layer increase. The process of diffusion under strain condition is an important factor that helps to understand reorientation process in molecular dynamics simulation. The mechanism behind the nitrogen diffusion in iron under strain condition at the level of nanoscale is still unclear. The purpose of the present work is to provide a molecular simulation of nitrogen diffusion model, which describes the nitrogen distribution in bcc iron during strain process. The iron–nitrogen nanocrystalline is generated and this system is subjected to tensile and compression strain along [1120] and [0001] directions of iron at different temperatures.

2. Theory and computational methodology

2.1. Molecular dynamics method

MD is a powerful tool for modeling motions of particles in a given system to determine positions, velocities and forces of each particle at every time step. In this study, LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator), Developed at Sandia National Laboratories, is utilized to run MD simulations on parallel computers [24].

The Modified Embedded-Atom Method (MEAM) potential, firstly proposed by Baskes in 1992, is used to describe the interactions between atoms in this MD simulation [25].

MEAM is an interatomic potential formalism applicable to a wide range of materials. The total energy, E , of a system of atoms in the MEAM formulation is given by [24].

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

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

A bcc super-cell of 3200 iron atoms including 50 randomly distributed nitrogen atoms in a three-dimensional box with edge lengths of $L_x = 16 \text{ nm}$, $L_y = 10 \text{ nm}$, $L_z = 10 \text{ nm}$ is considered. Periodic boundary conditions are applied on the boundaries so that the total number of atoms is maintained constant during the simulation. In order to investigate the strain diffusion process, nitrogen atoms are placed in a spherical hole inside the iron box. The radius of this spherical hole is $1 \text{ \AA}$ which is placed in the center of simulation box. Fig. 1 shows the atomic structure of simulated system. The structure is then minimized until the pressure and energy of the system reach a minimum value. Then, the structure is equilibrated at desired temperature.

The interatomic interactions are described with MEAM formulation. The potential parameters for Fe–N system are built according to the 2NN-MEAM developed by Lee et al. [26] for pure Fe and N. These parameters are modified in the 2NN-MEAM library file and introduced in LAMMPS.

A random velocity is assigned for each particle corresponding to Maxwell distribution at a desired temperature. The Velocity-Verlet algorithm is utilized to track the motions of interacting particles and numerically update the particle's phase-space trajectories. MD simulations are carried out using a microcanonical ensemble in which a constant NVE integration is

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