



Grain boundary and lattice diffusion in nanocrystal α -iron: An atomistic simulation study



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HIGHLIGHTS

- MD simulations were performed to find pure grain boundary diffusivity in nanocrystalline iron with grain size of 2.5 nm.
- High diffusivity paths in nanocrystal samples were visualized at grain boundaries.
- A temperature-dependence of the diffusion coefficient according to the Arrhenius law was obtained.
- Enhanced diffusivity of iron atoms in nanocrystal iron was attributed to the mixing rule for pure lattice and grain boundary diffusion and decrease of activation energy.

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ABSTRACT

To obtain fundamental understanding on the effect of grain boundaries on the diffusion kinetics, molecular dynamics simulations (MD) were carried out on single crystal and nanocrystal (with a mean grain size of 2.5 nm) bcc iron using the second nearest-neighbor modified embedded atom method (2NN-MEAM) interatomic potential. Self-diffusion coefficient in single crystal and nanocrystal samples were calculated in the temperature range from 350 K to 1000 K. A temperature-dependence of the diffusion coefficient according to the Arrhenius law was obtained for both lattice and grain boundary diffusion. By doing so, activation energies as well as pre-exponential factors were derived from the diffusion coefficients and compared to experimental data. MD simulation results show that diffusion rate of iron atoms in nanocrystal sample is 6 to 28 orders of magnitude greater than single crystal. The trajectory of iron atoms during diffusion process verified that diffusion occurs mostly in the grain boundaries of nanocrystal iron; suggesting that grain boundary diffusion is dominant in nanocrystal iron. Based on the obtained results pure grain boundary diffusion coefficient was calculated.

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1. Introduction

Iron and iron-based alloys are important commercial materials which often are used at temperatures where diffusion process strongly affect their properties [1,2]. Many metallurgical processes such as, homogenizing, aging, corrosion, precipitation, creep and diffusion bounding are diffusion process and significant changes in mechanical and physical properties can occur by diffusion [3–6]. In order to estimate and control the microstructure of poly-crystalline iron-based alloys a quantitative understanding of self-diffusion behavior of iron is important.

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Self-diffusion in poly-crystal solids can occur through lattice or lattice defects such as dislocations, grain boundaries (GB) and free surfaces [7–9]. Among lattice defects, grain boundaries provide the most prominent high-diffusivity paths and play a crucial role in diffusion process of many poly-crystals [7]. In particular, in nanocrystalline materials which are poly-crystals whose grain sizes are smaller than several hundred nanometers [8], grain boundary diffusion is a transport phenomenon of fundamental and technological importance [7]. Knowledge and understanding of grain boundary diffusion is vital in nanocrystalline materials science because, mass transfer will be even higher than in microcrystalline materials due to the large fraction of atoms (as high as 50% in some cases) in the grain boundaries [9].

Diffusion along grain boundaries often controls the evolution of the microstructure and properties of nanomaterials at elevated temperatures [10]. In processes such as Coble creep, sintering, diffusion induced grain boundary motion, discontinuous reactions, recrystallization and grain growth, diffusion along grain boundaries plays a prominent role [11].

A few experimental studies are available for self-diffusion coefficient in body centered cubic (bcc) iron with microcrystalline structures (grain size $< 1 \mu\text{m}$) for a wide range of temperatures [12–15]. However quantitative experimental knowledge on pure grain boundaries diffusivities in polycrystalline materials are still unknown. Because, in experimental measurements of lattice and grain boundary self-diffusion coefficients the influence of high diffusivity paths is unwanted [16]. Two major factors determine the quality of diffusion measurements, the method used and the extent to which the sample material is characterized [17]. The importance of specifying the material cannot be overstated. The measured diffusivity depends apart from the chemistry of the sample on its microstructure. Dislocations and grain boundaries can lead to apparent values of the diffusivity that are usually larger than the true lattice value. The promising accurate method to overcome the mentioned difficulties is atomistic simulations, using proper inter-atomic potentials [18]. Among various simulation techniques available in the literature [19,20], molecular dynamics (MD) simulation was found to be ideal for the estimation of mechanical (fatigue, fracture and creep) and physical (diffusion coefficient) properties [21].

F. Yuan [22] and K. Kadau et al. [23] have studied the mechanical properties of bulk nanocrystalline bcc iron and aluminum metals under tensile deformation by molecular dynamics (MD) simulations, respectively; and they found an inverse Hall–Petch relation for the flow stress for grain sizes smaller than 10–13.54 nm. S. Banerjee and et al. [24] calculated the surface self-diffusion coefficient of Sn atoms in the plane of grain boundary at 400 K for pure Sn system and for Sn alloys with In and Pb dopant atoms by molecular dynamics simulation. They reported that the self-diffusion coefficient of Sn atoms at the grain boundaries is more than an order of magnitude larger than lattice diffusion. Michael S. Sellers and et al. [25] computed the grain-boundary self-diffusion coefficient in five β -Sn symmetric tilt grain boundaries using MD simulations and they found that grain boundary with high excess potential energy exhibited larger diffusive widths.

Recently Mikhail L. Mendeleev and et al. [26] have calculated the lattice diffusivity in bcc iron assuming the vacancy and interstitial mechanism of self-diffusion by molecular dynamics simulations. Y.-J. Wang and et al. [27,28] reported a molecular dynamics analysis of creep in nanocrystal copper and found that the dominating creep mechanism transits from grain boundary (GB) diffusion to GB sliding, and then dislocation nucleation with increasing stress. Also, large-scale atomistic modeling is applied by Y.-J. Wang and et al. [29] to understand the diffusion kinetics in nanocrystalline copper.

Although a significant amount of molecular dynamics simulation work has been reported on grain boundaries in various materials and alloys; however, to the best of author's knowledge, there are few computational research studies on pure grain boundary diffusivity in bcc iron (ferrite phase). In order to calculate the pure grain boundary diffusivity in nanocrystal iron samples, the influence of lattice diffusion should be very small. Therefore, in the present study MD simulations were performed on nanocrystal sample with small grain size of 2.5 nm and high volume fraction of grain boundaries (about 55%). It should be noticed that average grain size of 2.5 nm cannot be achieved by experimental methods. Also to compare grain boundary diffusion with that of lattice diffusion, a single crystal iron sample with the same dimension as nanocrystal sample was generated and the effect of grain boundaries on the diffusion coefficient is investigated for different temperatures. The method used for generation of initial single crystalline and nanocrystalline structure and the computational model used in MD simulations are briefly described in Section 2.

2. Computational details

2.1. Molecular dynamics simulations

MD simulations were performed using the large-scale atomic/molecular massively parallel simulator (LAMMPS) open source code [30] and second nearest-neighbor modified embedded atom method (2NN-MEAM) interatomic potential [31,32]. Before each calculation for diffusion process, 2NN-MEAM interatomic potential for iron was valid by calculating certain physical properties of the iron system such as bulk modulus and elastic constant. Since there are experimental data on bulk modulus and elastic constant of bcc iron, the corresponding physical properties were calculated by MD simulation in this study to compare calculated results with experimental data. For inter-atomic potential validation, a super cell with $15 \times 15 \times 15$ unit cells consisting of 6750 atoms was considered. Periodic boundary conditions were applied along x , y and z directions of the unit cell. The system was equilibrated using NPT (constant pressure and temperature) ensemble at 300 K under pressure of 1 bar. Equilibrium value for lattice constant was assumed as 2.855 Å. The lattice parameter was varied from 2.855 to 2.860 Å and variation in the potential energy was monitored as a function of lattice constant for every 30 ps

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