DIFFUSION OF He INTERSTITIAL AND SMALL CLUSTERS AT GRAIN BOUNDARIES IN α-Fe—

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EXTENDED ABSTRACT (submitted to the Journal of Nuclear Materials as part of the proceedings of the 12th International Conference on Fusion Reactor Materials, Santa Barbara, California, December 4–9, 2005)

A systematic molecular dynamics study of the diffusion mechanisms of He interstitial and their small clusters at two representative interfaces, Σ11 and Σ3, has been carried out in α-Fe. The diffusion coefficient of a He interstitial and the effective migration energies were determined, and the diffusion mechanisms of single interstitials and di-He interstitials are discussed in detail. A di-He interstitial cluster can kick out a self interstitial atom (SIA) at high temperatures, forming a He_2V complex. The SIA migrates rapidly near interfaces, whereas the He_2V complex is immobile at the temperatures considered. This small cluster may serve as a smallest nucleation for the formation of helium bubbles at interfaces.

Most of the details pertaining to the methodology used in the calculations of the atomic arrangements of GBs have been described in detail elsewhere [1,2]. Two symmetric tilt GBs, Σ3 {112} Θ = 70.53°, Σ11 {323} Θ = 50.48°, were employed to study diffusion of He interstitials and small clusters in the temperature range from 600 to 1200 K. The interatomic potentials used in this research have been described in detail previously [3]. The migration simulations were followed for 1–14 ns, depending on the temperature. The diffusivity, D, of He atoms can be determined from the sum of the mean square displacements (MSD) of He atoms. To accurately calculate the diffusion coefficient of He atoms, the method used here is based on decomposing the single trajectory into a set of shorter independent segments with equal duration, and then an average MSD, D_i (i indicates the ith time interval for the segment) for each segment is calculated. The time interval of segments varies from 10 ps to 500 ps, and then D_i is averaged over all time intervals. With the diffusion coefficients of He atoms obtained at different temperatures, the activation energy for He migration in GBs, E_m, can be estimated from the Arrhenius Relation where D_0 is the pre-exponential factor and k_β is the Boltzmann constant.

$$D = D_0 \exp\left(-\frac{E_m}{k_\beta T}\right), \qquad (1)$$

The mean square displacements of a He interstitial are determined as a function of time for the Σ3 and Σ11 GB using the method described above. During the simulation, a large number of He jumps are observed, but the dynamic processes occasionally involve the jumps of Fe atoms. However, the contribution of Fe jumps to the total MSD is negligible. The diffusion coefficients estimated for the He interstitial in both GBs are given in Fig. 3 as a function of reciprocal temperature, where circle symbols represent the data calculated for the Σ3 GB and square symbols indicate the data obtained for the Σ11 GB. The data approximately follow an Arrhenius relationship, from which the corresponding activation energies, E_m, and pre-exponential factors, D_0, can be determined. The best fits of these results to Eq (1) give the values of E_m and D_0 to be 0.28 eV and $4.39\text{x}10^{-4}\text{cm}^2/\text{s}$ for the Σ3 GB, and 0.34 eV and 4.3 $\text{x}10^{4}\text{cm}^2/\text{s}$ for the Σ11 GB, respectively.

The migration mechanisms of He interstitials in GBs have been studied by analysis of the computer-generated trajectories. The result suggests that the He interstitial mainly migrates with one-dimensional behavior at low temperature. However, it has been observed that the migration path of the He interstitial changes from one-dimensional (1D) diffusion to two-dimensional (2D) diffusion in the interface plane at

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