NUMERICAL SIMULATION OF HYDROGEN ENTERING A SECOND PHASE PARTICLE IN ALUMINUM

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High-strength aluminum (Al) alloy has been developed as a structural material for automobiles and aircraft. Such an alloy is beneficial for reducing their total weight while maintaining their strength. However, as the alloy becomes stronger, the susceptibility to hydrogen embrittlement (HE), which brings about a loss of ductile and/or crack formation, becomes more remarkable. It is known that HE occurs when H atoms gathering at the part of stress concentration in the alloy are trapped by the interface defects such as grain boundaries and phase interfaces and weaken the atomic bond. Therefore, it is considered that the occurrence of HE can be suppressed by decreasing H atoms trapped by such interface defects. Recently, it is indicated by first-principles calculation that the second particle of tin (Sn) in Al can trap H atoms on the inside, and it is shown experimentally that the loss of ductility by H atoms is suppressed in the Al-Zn-Mg alloy when added Sn [1]. Thus, in this study, by simulating H entering the inside of an Sn particle in the Al matrix, we examined the H partitioning between the inside of the Sn particle and the interface between the Sn particle and the Al matrix. The model obtained by modifying the model proposed by Enomoto [2] for simulating thermal desorption spectra of H from ferrite-austenite dual-phase steels was employed as the simulation model. That was represented by the one-dimensional reaction-diffusion equation for the radial direction in a polar coordinate. We used the diffusion coefficient of H in Sn and Al which is reported experimentally. Figure 1 shows an example of the simulation result. We discuss the possibility of suppressing HE by adding Sn to the Al alloy on the basis of the simulation results.

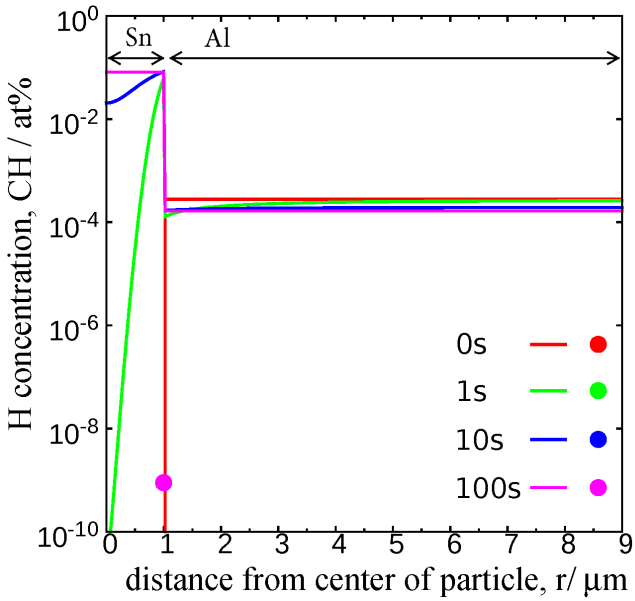

Figure 1 Example of simulation of H entering the Sn particle: The symbol means the concentration of the interface trap site. The case that the H trapping energy is 50 kJ/mol and the trap site concentration is 5.4×10^{19} /m^3 is shown. The symbol means the H concentration of the interface trap site.

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Reference

[1] B. Sharma, submitted.
[2] M. Enomoto, International Journal of Hydrogen Energy 42(2017)10579