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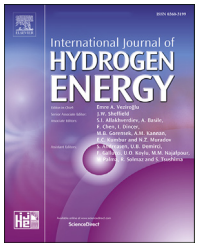

The effect of Na addition on the first hydrogen absorption kinetics of cast hypoeutectic Mg–La alloys

Manjin Kim [a,*], *Qinfen Gu* [b], *Tanveer Hussain* [c], *Yahia Ali* [a], *Trevor B. Abbott* [a,d,e], *Kazuhiro Nogita* [a]

[a] *School of Mechanical and Mining Engineering, The University of Queensland, Brisbane, Queensland, 4072, Australia*

[b] *Australian Synchrotron, ANSTO, Clayton, Victoria, 3168, Australia*

[c] *School of Chemical Engineering, The University of Queensland, Brisbane, Queensland, 4072, Australia*

[d] *School of Engineering, RMIT University, Carlton, Victoria, 3053, Australia*

[e] *Magontec Ltd., Sydney, New South Wales, 2000, Australia*

HIGHLIGHTS

- Na additions to Mg–La alloys does not change the microstructure of the alloys.
- Na additions improve H_2 absorption kinetics of Mg–La alloys.
- No significant effect of microstructure change on H_2 absorption is confirmed.
- The surface of Na doped Mg–La alloy shows a stronger adsorption energy of H_2.

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ABSTRACT

With superior properties of Mg such as high hydrogen storage capacity (7.6 wt% H/MgH_2), low price, and low density, Mg has been widely studied as a promising candidate for solid-state hydrogen storage systems. However, a harsh activation procedure, slow hydrogenation/dehydrogenation process, and a high temperature for dehydrogenation prevent the use of Mg-based metal hydrides for practical applications. For these reasons, Mg-based alloys for hydrogen storage systems are generally alloyed with other elements to improve hydrogen sorption properties. In this article, we have added Na to cast Mg–La alloys and achieved a significant improvement in hydrogen absorption kinetics during the first activation cycle. The role of Na in Mg–La has been discussed based on the findings from microstructural observations, crystallography, and first principles calculations based on density functional theory. From our results in this study, we have found that the Na doped surface of Mg–La alloy systems have a lower adsorption energy for H_2 compared to Na-free surfaces which facilitates adsorption and dissociation of hydrogen molecules leading to improvement of absorption kinetic. The effect of Na on the microstructure of these alloys, such as eutectic refinement and a density of twins is not highly correlated with absorption kinetics.

* *Corresponding author.*
E-mail address: manjin.kim@uq.net.au (M. Kim).

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