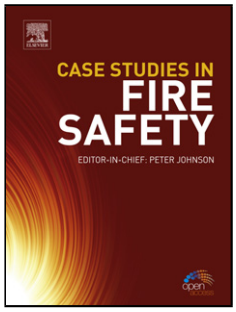

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An experimental and theoretical study of the hydrogen resistance of Ti_3SiC_2 and Ti_3AlC_2

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Highlights

- Hydrogenation leads to significant structure degradation on Ti_3AlC_2 by promoting the exudation of Al atoms which form Al bubbles on the powders surface, while there is no obvious morphology change on Ti_3SiC_2.
- The more apparent hydrogen-induced degradation observed for Ti_3AlC_2 is theoretically interpreted by the higher hydrogen diffusivity in Ti_3AlC_2 and the larger reduction of both formation energy and diffusion energy barrier of Al vacancy in Ti_3AlC_2 than corresponding values of Si vacancy in Ti_3SiC_2.

Abstract: The hydrogen resistance of Ti_3SiC_2 and Ti_3AlC_2 is investigated by a combination of high temperature hydrogenation experiments and first-principles calculations. The hydrogen absorption rate in Ti_3AlC_2 powders is twice of that in Ti_3SiC_2. Hydrogenation leads to significant structure degradation on Ti_3AlC_2 by promoting the exudation of Al atoms which