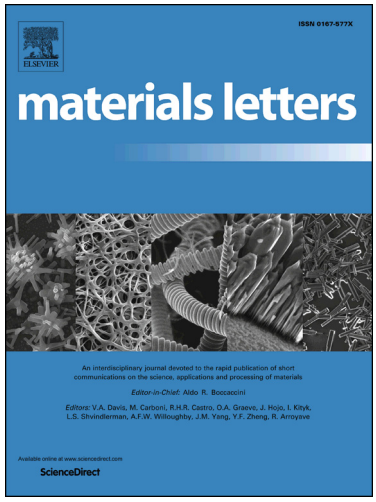

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Effect of local stress on hydrogen segregation at grain boundaries in metals

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Abstract

Hydrogen embrittlement (HE) has been a consistent obstacle in the design of reliable structural metals. In search of ways to mediate HE susceptibility of metals, grain boundary (GB) engineering emerges as an effective means. Here, atomic simulations were carried out to investigate the critical role of stress in hydrogen segregation at GBs in several representative metal systems. The hydrostatic stress is shown to be directly responsible for local volumetric distortion at individual polyhedrons that constitute GBs, confirming its significance in determining hydrogen adsorption energetics. Our findings provide new clues towards micromechanical modeling of hydrogen-GB interactions.

Keywords: Hydrogen embrittlement; grain boundaries; segregation; local stress.

Hydrogen embrittlement (HE), a daunting phenomenon of structural metals suffering premature failure as a consequence of the presence of hydrogen, has haunted many

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