

学术报告

题目: Helium Trapping in Nano-Structured Ferritic Alloys: a First Principles Study

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报告摘要:

Y2Ti2O7 and Y2TiO5 are two primary precipitate phases in nano-structured ferritic alloys (NFAs). We report a first-principles study on the selective trapping of helium in nano-size oxides in NFAs. Calculation results suggest that (1) compared to vacancy sites in the iron matrix, the radiation induced helium prefers the octa-interstitial sites in Y2Ti2O7 and the the b-axis open-channel of Y2TiO5. (2) The He-He interaction in Y2Ti2O7 is essentially repulsive. Helium dispersion would largely depend on the number and dispersion of oxide particles in NFAs. (3) Charge transfer occurs only between helium and neighboring oxygen anions, suggesting the generality of trapping helium in oxides. (4) Helium segregation to the Fe/Y2Ti2O7 interface may sensitively depend on the size of oxide particles. These fundamental results provide profound new insights into the behavior and management of helium in NFAs, including: (1) helium is first deeply trapped in oxides and their interfaces; (2) energy of helium is lower in bubbles than in the oxide when the bubbles are above a critical size; (3) bubbles nucleate at the interfaces and grow by bleeding of helium from the oxides and a continued flux from the matrix; (4) the size of the bubble correlates with the size of the oxide and its helium content; (5) bubbles can remain small in the case of a fine distribution of nm-scale oxides, effectively managing helium by storing it at high pressure; (6) a corollary is that larger-sized oxides form larger-sized, lower pressure bubbles that may be harmful, for example, by serving as formation sites for growing voids. All these results are incorporated in a microstructure-based multiscale, thermo-kinetic model of helium transport, fate, and consequences.

报告人简介:

江勇, 中南大学材料学院教授, 博士生导师。1995年本科毕业于中南工业大学, 1998年获硕士学位(材料加工力学), 2004年在美国亚利桑那州立大学获硕士学位(固体电子学), 2005年获博士学位(计算材料学)。2000-2005年, 先后在美国克莱姆森大学和亚利桑那州立大学从事助研、助教工作, 2005年4月起在美国德尔福研究所任材料工程师, 2007年1月起在美国加州大学圣芭芭拉分校任博士后学者, 2008年9月-10月在英国剑桥大学工作访问, 2009年6月起在美国加州大学圣芭芭拉分校任研究副专家。2010年11月被聘为中南大学“升华计划”特聘教授。长期专注于材料表面与界面相关结构与性能的基础性研究, 及其在新一代航空发动机高温涂层、新型核电用钢、合金与金属基复合材料、功能氧化物等领域的应用。在 Acta Mater、Scripta Mater、Phys Rev B、Appl Phys Lett、J Phys Chem B、RSC Advances、Phys Chem Chem Phys、J Chem Phys、J Appl Phys、Chem Phys Lett、Philo Magz、J Mater Sci 等国际知名期刊发表论文 31 篇, SCI 单篇最高他引 88 次。现担任美国《Metall Mater Trans E》期刊 Key Reader, 美国物理学会期刊《Phys Rev B/Lett》常年评审, 以及《Nanoscale》等 10 余种国际期刊通讯审稿人。