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The effect of Cr concentration on displacement cascades in Fe-Cr binary alloys

Xinhua Yang

Huazhong University of Science and Technology, China

Displacement cascades in random Fe-Cr binary alloys with a wide range of Cr concentration from 2% to 20% were simulated by using the molecular dynamics method and the effect of Cr concentration on cascade damage was carefully investigated. The results showed that the average number of surviving Frankel pairs is approximately the same in Fe-Cr alloys and the average fraction of vacancies in clusters is roughly constant, within scatter, over the whole range of Cr concentration. The average fraction of self-interstitial atoms (SIAs) is slightly bigger in a lower Cr concentration alloy than in a higher Cr concentration alloy. The number of Cr atoms associated with survived self-interstitial defects was analyzed. The data show that the content of Cr in interstitials approximately exceeds two or three times the matrix content, which indicated that there is a significant enrichment of SIA defects by Cr.

Recent Publications

1. Malerba L, Bonny G, Terentyev D, Zhurkin E E, Hou M, Vörtler K and Nordlund K (2013) Microchemical effects in irradiated Fe-Cr alloys as revealed by atomistic simulation. *Journal of Nuclear Materials* 442:486-498.
2. Tikhonchev M, Svetukhin V, Kadochkin A and Gaganidze

E (2009) MD simulation of atomic displacement cascades in Fe-10 at.%Cr binary alloy. *Journal of Nuclear Materials* 395:50-57.

3. Vörtler K, Björkas C, Terentyev D, Malerba L and Nordlund K (2008) The effect of Cr concentration on radiation damage in Fe-Cr alloys. *Journal of Nuclear Materials* 382:24-30.
4. Björkas C, Nordlund K, Malerba L, Terentyev D and Olsson P (2008) Simulation of displacement cascades in Fe90Cr10 using a two band model potential. *Journal of Nuclear Materials* 372:312-317.
5. Shim J H, Lee H J and Brian B D (2006) Molecular dynamics simulation of primary irradiation defect formation in Fe-10%Cr alloy. *Journal of Nuclear Materials* 351:56-64.

Biography

Xinhua Yang working as full time professor at Huazhong University of Science and Technology, Wuhan, China

yangxinh@hust.edu.cn