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Disorder trapping during crystallization of the B2 ordered NiAl system DEYAN SUN, XIAOQING ZHENG, YANG YANG, YUFENG GAO, Department of Physics, East China Normal University, Shanghai 200062, China, JEFF J. HOYT, Department of Materials Science and Engineering, McMaster University, Hamilton, ON, Canada, MARK ASTA, Department of Materials Science and Engineering, University of California, Berkeley, CA 94720 — Using molecular dynamics (MD) simulations, disorder trapping associated with solidification is studied for the (100), (110) and (111) growth directions in the B2 NiAl ordered alloy compound. At the high interface velocities studied we observe pronounced disorder trapping, i.e., the formation of antisite defects and vacancies in the crystal at higher than equilibrium concentrations upon rapid solidification. The vacancies are located primarily on the Ni sublattice and the majority of antisite defects are Ni atoms on the Al sublattice, while the concentration of Al on the Ni sublattice is negligibly small. The defect concentration is found to increase in an approximately linear relationship with an increase of the interface velocity or undercooling. Further there is no significant anisotropy in the defect concentrations for different interface orientations.

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