Nanoscale Patterning of L1$_2$ Chemical Order in Ni$_3$Al Alloy Processed by Energetic Ions

JIA YE, YOUHONG LI, ROBERT AVERBACK, PASCAL BELLON, JIANMIN ZUO — We recently predicted that alloys forming chemical ordered phases at equilibrium can be forced into stable nanoscale patterns of chemical order by irradiation with energetic particles. We have tested this prediction on the Ni$_3$Al compound by combining MD and KMC simulations. For 1MeV Kr and 70KeV He ions, MD simulation is used to simulate the disordered zones, which are then incorporated into KMC simulations to reach long irradiation times. We introduce a new method based on scaling behavior of structure factor to identify reliably the transition boundary between patterning and disordered states. These simulations indicate that 1MeV Kr ion irradiation can lead to patterning, whereas 70KeV He ion cannot. These results are compared to experimental results, obtained by performing ion irradiations on Ni$_3$Al thin films grown by sputtering.