Surface segregation in bcc-based Fe-Al and Co-Al alloys: The role of bulk-like ordering interactions

V. Blum, L. Hammer, W. Meier, O. Wieckhorst, S. Müller, K. Heinz
Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg
Staudtstr. 7, 91058 Erlangen, Germany
v.blum@fkp.physik.uni-erlangen.de

We have performed detailed crystallographic analyses of (100)-oriented surfaces of bcc-based $Fe_{1-x}Al_x$ ($x = 0.03, 0.15, 0.30, 0.47$) and B2 CoAl by means of quantitative low-energy electron diffraction (LEED). The results are interpreted in terms of a simplified model of SRO in both systems, underpinned by some very recent *ab initio* calculations. In $Fe_{1-x}Al_x(100)$, Al segregates, with in-plane 2NN ordering forces "shaping" the compositional development of the topmost atomic layer as a function of x. CoAl(100) also terminates with its (nominal) Al sublattice, but the topmost layer here contains an unexpected amount of ≈ 30 % Co antisite defects. We explain this by much stronger bulk NN interactions in this system, which drive a small amount of residual, sputter-induced Co antisite defects in the near-surface region out to the very surface. It is our central result that the properties of bulk structural defects may dominate the surface behaviour of strongly ordering, near-stoichiometric binary alloys.