Segregation and Ordering at the (110) Surface of Ni-rich NiAl

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Abstract – Various surfaces of Ni-rich NiAl show an enhanced concentration of Al in the first surface layer. Our synchrotron experiments for the (110) surface of $Ni_{90}Al_{10}$ also revealed that the surface layers are ordered while the underlying bulk is disordered. In order to understand this observed behavior we have investigated the system using an ab-initio based Cluster Expansion. It turns out that segregation and ordering at the surface is driven by changes in the electronic structure induced by the surface. The modified bonding behavior in the surface can be understood in a tight-binding description using the invariant covalent bond energy.