Surface phase diagram of CoAl(100)

O. Wieckhorst[1], S. Müller[1], L. Hammer[1], K. Heinz[1], R. Drautz[2], M. Fähnle[2]

[1] *University Erlangen-Nürnberg, Lehrstuhl für Festkörperphysik, Staudtstr. 7, D-91058 Erlangen*
[2] *Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart*

The combination of density functional theory (DFT) [1] with concepts from statistical physics is applied to construct a DFT-based phase diagram for a binary alloy surface without any empirical parameters. While treating the results of DFT calculations within a thermodynamic model reveals the stable ordered phases, application of a cluster expansion [2] in conjunction with Monte Carlo simulations allows to treat short range order in the alloy surface.

As an example, we studied the structure and stability of the B2-CoAl(100) surface consisting of alternating Co- and Al-layers. For ideal bulk stoichiometry, the (100)-surface shows a termination by the Al-sublattice. However, as we have recently shown [3], a tiny surplus of Co-atoms in the bulk leads to the formation of antisite atoms, i.e. Co-atoms on the Al-sublattice, which segregate to the surface. The observed ordering strongly depends on the density of antisite atoms in the near surface region. Based on DFT calculations in combination with an appropriate thermodynamic model, it is possible to construct a phase diagram for the CoAl (100) surface, as shown in Fig 1. While still based on the assumption of a long range ordered surface, comparison of the structural parameters of the predicted stable phases are in quantitative agreement with those retrieved from LEED structure determinations [4, 5]. However, long range order is still assumed in the surface, and thus the model fails to describe short range order of the antisite atoms as observed for CoAl(100). Incorporating short range order into modelling an alloy surface requires both, the treatment of large unit cells containing thousands of atoms and a method for scanning configuration space [7, 6]. The limitations of our model, which is based only on long range ordered DFT calculations, can be overcome by combination of the DFT calculations with a cluster expansion (CE) and Monte-Carlo (MC) simulations. This approach considers both layer dependent interactions and configurational entropy. Thus, we can study ordering phenomena and segregation profiles of metal alloy surfaces.

For the CoAl surface a competition between ordering behaviour in the first layer and clustering of Co-atoms in the third layer is induced by the interlayer interactions. This results in a change of the type of ordering in the first layer with increasing Co-concentration in the third layer. This change is demonstrated using layer-resolved short range order parameters. The change in ordering of the first layer and the stable structures predicted are in excellent agreement with experiment.

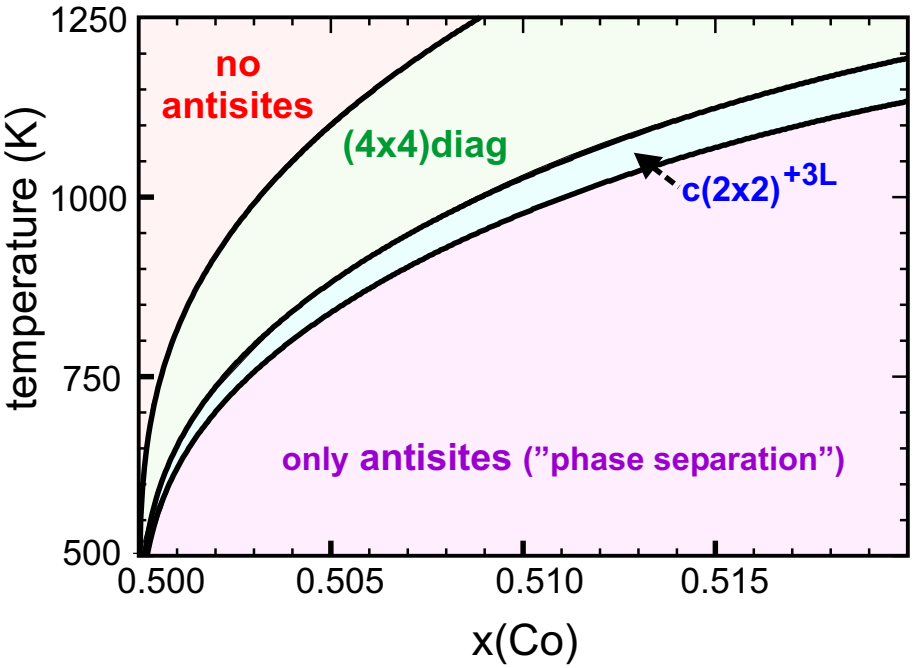

Figure 1: Surface phase diagram of the CoAl(100) surface

References

[1] Kresse G and Furthmüller J 1996 *Phys. Rev. B* **54** 11169; 1996 *Comput. Mater. Sci.* **6** 15

[2] J. M. Sanchez, F. Ducastelle, D. Gratias, Physica A **128**, 334 (1984).

[3] V. Blum, L. Hammer, Ch. Schmidt, W. Meier, O. Wieckhorst, S. Müller, and K. Heinz, Phys. Rev. Lett. **89**, 266102 (2002).

[4] O. Wieckhorst, S. Müller, L. Hammer, and K. Heinz, subm. to Phys. Rev. Lett.

[5] V. Blum and K. Heinz, Comp. Phys. Comm. **134**, 392 (2001). subm. to Phys. Rev. B

[6] S. Müller, J. Phys.: Condens. Matter **15**, R1429 (2003).

[7] R. Drautz, H. Reichert, M. Fähnle, and H. Dosch, J. M. Sanchez, Phys. Rev. Lett. **87**, 236102-1 (2001).