	Experiment title: Surface Induced Order at $Cu_{1-x}Pd_x(001)$ Surfaces	**Experiment number**: SI 772
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Report:

In previous experiments we have detected surface induced order (SIO) for the alloys $Cu_{75}Pd_{25}(001)$ and $Cu_{80}Pd_{20}(001)$ [1]: A surface layer remains ordered up to a temperature $T_{0,S}$ above the bulk order-disorder phase transition temperature $T_{0,B}$. In the case of $Cu_{75}Pd_{25}$ the SIO is extremely stable ($T_{0,S}-T_{0,B}\sim405K$). Barbier et al. [2] demonstrated clearly that $Cu_{83}Pd_{17}(001)$ exhibits surface induced disorder (SID). The following table summarizes the situation:

Composition	$T_{0,S}-T_{0,B}$ [K]	Type of surface phase transformation	Remarks
$Cu_{83}Pd_{17}$	0	SID	[2]
$Cu_{80}Pd_{22}$	10	SIO	[1] SI 663
$Cu_{75}Pd_{25}$	405	SIO	[1] APS and this experiment

For $Cu_{80}Pd_{20}$, we were able to deduce a detailed model for the composition and order parameter profile in the surface region at temperatures above $T_{0,B}$. In this experiment we reinvestigated the $Cu_{75}Pd_{25}$ sample which shows the extremely stable SIO in order to get a clear picture of its surface structure, as we did for $Cu_{80}Pd_{20}$.

The polished surface of the single crystal sample was prepared by cycles of Ar sputtering and annealing. The absence of contaminants was verified by Auger electron spectroscopy. The sample was mounted horizontally in a mobile UHV-chamber. The diffraction experiments were performed at an energy of 17.12 keV (0.7243 ≈ wavelength) in a grazing incidence geometry.

We confirmed the observation of extremely stable SIO. We are now able to pin down $T_{0,S}$ to $T_{0,B}$ + (405±20)K. **Figure 1** shows the integrated intensity of superstructure peaks around the equivalent positions (011) and (101) as a measure for the surface order (measured in surface sensitive grazing incidence geometry) and bulk order (measured with large incident angles). The actual positions are shifted because of peak splitting due to long period superstructures.

The (20L) fundamental and (10L) superstructure crystal truncation rods were measured at different temperatures above $T_{0,B}$. They allow a detailed analysis of the composition and order parameter profiles normal to the surface.
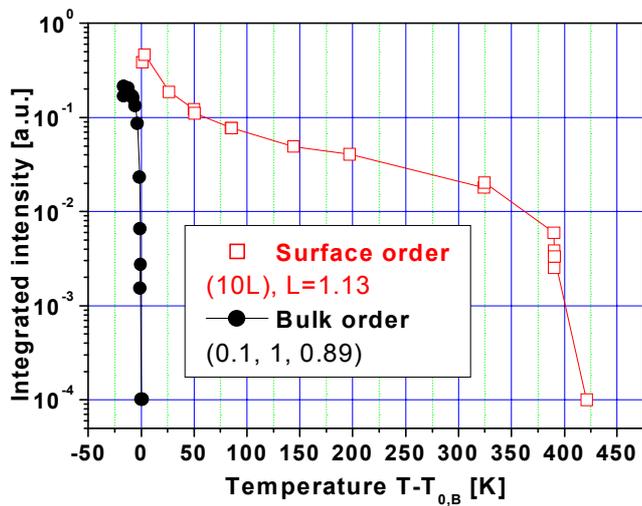
Figure 1: Integrated intensity of superstructure peaks characteristic for surface order (squares, measured in surface sensitive grazing incidence geometry) and for bulk order (circles, measured with large incident angles). The surface order persists up to temperatures of ~405 K above the phase transition temperature of the bulk.

The measurement of the (20L) rods permits to deduce the composition profile normal to the surface as described in [3]. **Figure 2** shows examples of such rods for different temperatures above $T_{0,B}$. The dip at the anti-Bragg position is attributed to an oscillatory composition profile with a Cu-rich first layer and an exponential damping (see topmost curve). For temperatures closer to $T_{0,B}$ additional features on the rod appear, that can be explained by the presence of buried antiphase domain boundaries. As $T_{0,B}$ and thus the fully ordered state is approached, the composition profile becomes more pronounced: The dip at the anti-Bragg position develops into a peak.

The (10L) rods give access to the in-plane order of the surface region. **Figure 3** shows (10L) rods for two different temperatures. The peaks (at L=0, 1, 2, ...) on the superstructure rod are split normal to the surface. This splitting shows the presence of antiphasing in the laterally ordered layer. It is <u>not</u> due to short range order. The in-plane width of the superstructure rod indicates a coherence length of the lateral order of up to $1000 \approx$.
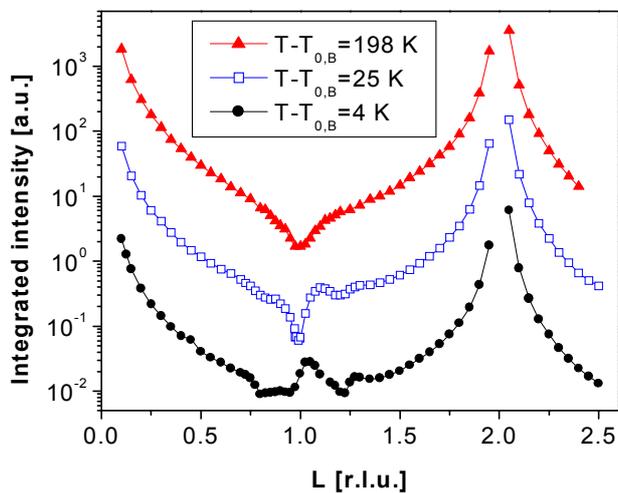
Figure 2: (20L) rods at different temperatures
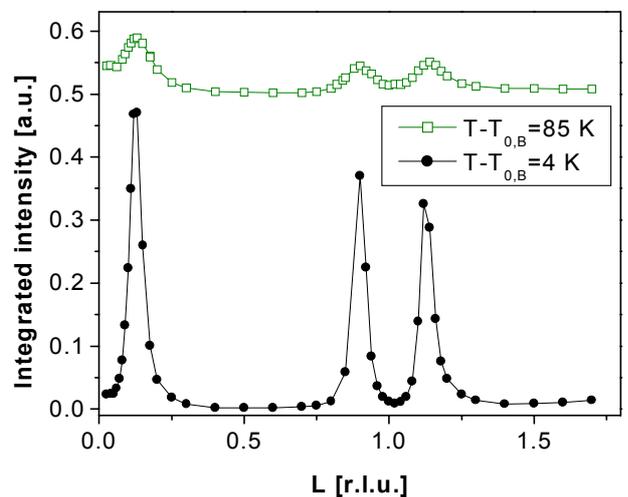
Figure 3: (10L) rods at different temperatures

A detailed modelling of the composition and order parameter profiles normal to the surface is currently in process. The results obtained for the different compositions so far show for the first time a transition from SID to SIO as a function of composition, thereby elucidating the role of the surface field h_1 and modified surface interaction parameters onto the nature of the surface phase transformation.

[1] H. Reichert, S. Engemann, C. Mocuta, W. Schweika, in preparation.
[2] L. Barbier et al., Phys. Rev. Lett. **78** 3003 (1997).
[3] H. Reichert, P. J. Eng, H. Dosch, I. K. Robinson, Phys. Rev. Lett. **74** 2006 (1995).