

Segregation and Ordering at the $\text{Cu}_3\text{Pd}(001)$ -Surface

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Introduction

Phase transitions at surfaces are often more complex than in the bulk. There exists a large body of literature describing in detail the thermodynamics of phase transitions at surfaces (see, e.g., these excellent reviews^{1,2}). In systems with a first-order bulk transition the most prominent surface transitions are surface-induced order (SIO) and surface-induced disorder (SID).³ Both types of surface phase transition have been clearly demonstrated in a still very limited number of systems.⁴⁻⁷

Methods and Materials

We have performed surface-sensitive x-ray diffraction measurements in order to determine the ordering behaviour and the related segregation phenomena at the $\text{Cu}_3\text{Pd}(001)$ -surface. Superstructure (10L) and fundamental (20L) crystal truncation rods (CTRs) at different temperatures above the bulk order-disorder transition temperature have been measured. Analysis of the CTRs allowed us to determine depth profiles of the order parameters and of the composition (i.e., segregation). The experiment has been carried out at the UNI-CAT beamline 33-ID using the surface experimental station which provides a six-circle diffractometer with an integrated ultrahigh vacuum (UHV) chamber.

The sample had previously been used in UHV for bulk scattering experiments. The (001)-surface was polished and cleaned by cycles of sputtering and annealing. It was found to be free of contaminations by Auger electron spectroscopy. The composition was verified by electron microbeam analysis.

Results

In our experiment, we found extraordinary stable surface induced ordering at the $\text{Cu}_3\text{Pd}(001)$ -surface. Whereas the bulk disorders at a transition temperature $T_{0,B}=733\text{K}$, a thin surface layer remains laterally ordered up to temperatures as high as about $T_{0,S}=1220\text{K}$ (see Fig. 1). Due to the low signal-to-background ratio and the limited number of temperature points, the nature of the surface transition remains unclear.

The thickness of the laterally ordered slab was determined by fitting the measured intensity profile of the superstructure (10L)-rod (see Fig. 2). This leads to a thickness of about 10 atomic layers with a gradual transition from the laterally ordered surface to the disordered bulk. The very small in-plane width of the superstructure rod indicates a large coherence length of about 1000\AA . The peaks on the superstructure rod are split normal to the surface. This is not due to short-range order but points to the presence of antiphasing in the ordered near-surface region.

Analysis of the fundamental (20L)-rod (see Fig. 3) revealed an oscillatory composition profile starting with a Cu-rich layer (about 5-11 at.-% enrichment depending on the temperature). The segregation profile is damped with a decay length of 3-5 atomic layers.

Discussion

In the most simple models for SIO, the transition temperature for the surface is determined by the ratio $V_{1,S}/V_{1,B}$ of the nearest

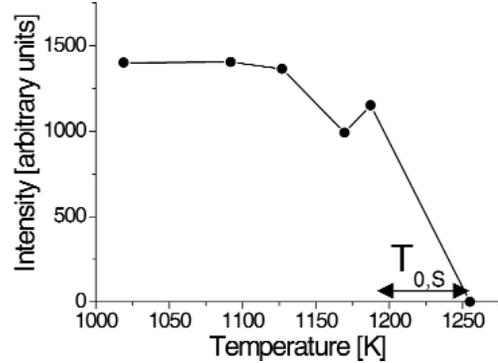


FIG. 1. Peak-intensity of the superstructure (10L)-rod.

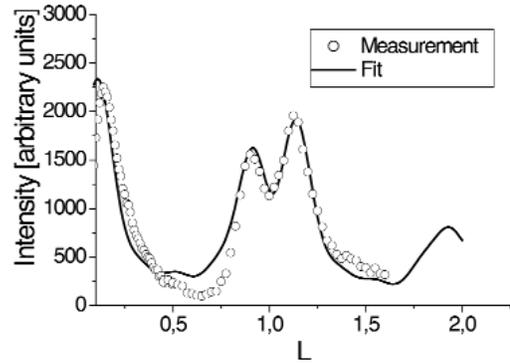


FIG. 2. Superstructure (10L)-rod at $T=1010\text{K}$.

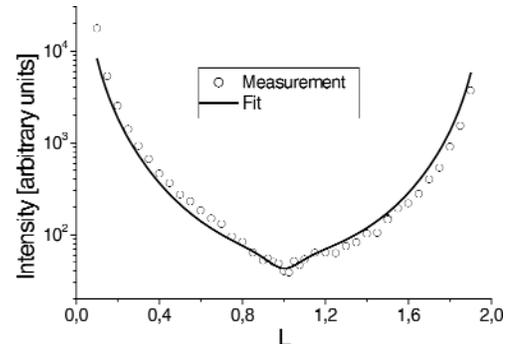


FIG. 3. Fundamental (20L)-rod at $T=1010\text{K}$

neighbour interactions in the surface and in the bulk. In order to explain $T_{0,S}/T_{0,B}$ having a value as large as 1.66, we have to assume a ratio of $V_{1,S}/V_{1,B}$ of the same order. This implies that the electronic structure at the surface should be quite different from the bulk for this system. Currently, the physical origin of the unprecedented strong surface induced ordering at $\text{Cu}_3\text{Pd}(001)$ is unclear. It is even more surprising since a very detailed study on a miscut $\text{Cu}_{83}\text{Pd}_{17}(001)$ -surface⁷ has clearly demonstrated SID. As the results on the segregation behaviour are in agreement, changes in the surface-ordering behaviour are induced by the concentration dependence of the interatomic potential rather than by a change of the surface energies.

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