| ESRF | **Experiment title:**<br>Temperature dependence of the short range order at a $Cu_3Au(001)$ surface | **Experiment number**:<br>SI-444 |
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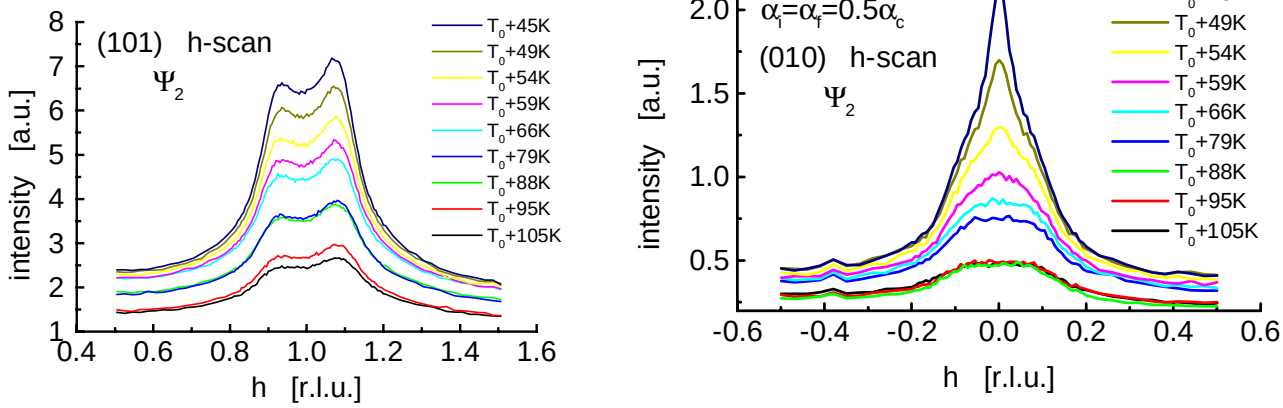
**Report:**

Diffuse scattering from disordered solid solutions is one of the major tools for the study of fundamental properties of these materials. The most important aspect of such measurements is the access to the local chemical order and effective pair interaction parameters as determined from the short range order (SRO) part of the diffuse scattering [1,2]. The fine structure of the SRO diffuse intensity, the so-called $k_F$-effects, reveals details about the electronic structure and entropy effects as well [3,4] and serves as the most important test for theoretical studies of alloy systems from first principles. In this experiment we have carried out a detailed measurement of the nature of short range order at the surface of a binary alloy. We have introduced the $Cu_3Au(001)$ single crystal into the stationary UHV chamber at the surface diffraction beamline. Previous experiments performed at the same sample have revealed the most detailed picture on ordering and segregation at this binary system [5-7], which could also be confirmed in this experiment.

In the experiment we have measured the bulk short range order along lines (1,k,1), (1+h,0,1) and (1,0,1+L) in a conventional wide angle scattering geometry, while measurements along (0,1+k,0), (h,1,0) and (0,1,L) at grazing angles allowed the determination of the symmetry of bulk and surface short range order at the same time. The measurements along (0,1+k,0) and (h,1,0) parallel to the surface have been performed for a set of different incident and exit

angles in order to study the depth dependence of the shape of the diffuse scattering (we have achieved a minimum scattering depth as low as 16Å!!). This set of measurements has been performed for 9 temperatures in the disordered phase which allows us to study entropy effects on the nature of the surface short range order as well. For all the measurements we have applied the most stringent control on incident and exit angle of the x-ray beam. In order to minimize background contributions we have used the analyzer setup at the surface diffraction beamline. The figures below show the bulk (left) and surface (right) diffuse scattering for various temperatures in the disordered phase. The split peak structure for the bulk clearly collapses into a central single peak at the surface




Since the fine structure of the diffuse scattering around superlattice positions, "$k_F$-effects", is determined by the electrons in the conduction band, the diffuse scattering experiment has shown the influence of surface electronic states on the nature of short range order in the disordered phase. Contrary to the bulk case, we found that "$k_F$-effects" in the surface short range order scattering are not present, i.e. correlations in the real space arrangement of fluctuating antiphase domains in the disordered phase are suppressed. Further modelling of the surface short range order is under way.


[1] S.C. Moss, Phys. Rev. Lett. **22**, 1108 (1969)
[2] D. de Fontaine, Solid State Physics **34**, 73 (1979)
[3] H. Reichert, S.C. Moss, K. S. Liang, Phys.Rev.Lett. **77**, 4382 (1996)
[4] H. Reichert, I. Tsatskis, S.C. Moss, Comp. Mat. Sci. **8**, 46 (1997)
[5] H. Dosch et al., Phys. Rev. Lett. **60**, 2382 (1988)
[6] H. Reichert, P.J. Eng, H. Dosch, I.K. Robinson, Phys.Rev.Lett.**74**, 2006 (1995)
[7] H. Reichert, P.J. Eng, H. Dosch, I.K. Robinson, Phys.Rev.Lett. **78**, 3475 (1997)