Atomic Steps on Surfaces

By Martin Henzler *

A special workshop on atomic steps at surfaces and interfaces (organized by *M. Henzler, W. Ranke* and *M. Scheffler*) was held at the Ringberg Castle in Rottach-Egern, FRG, from January 15–18, 1989. Due to the hospitality of the Max-Planck-Gesellschaft the participants from Germany (West and East), other European countries and the USA had an ideal meeting place for extensive discussions on an exciting topic.

In surface science in the past, surfaces have been frequently dealt with as if they were free of defects. This simplification was mainly due to the lack of reliable measurements of the defects and a lack of theory concerning deviations from periodicity. However, over the last twenty years, a few groups have developed defect analysis via profile analysis of diffraction spots. Other techniques, especially microscopy have contributed a lot, so that now the atomic step is the best investigated defect at surfaces. It was therefore worthwhile to put together all available information on steps with respect to verification, theory and properties into one workshop.

It was very helpful to have all the powerful structure elucidation methods reviewed, such as the various microscopies (transmission electron microscopy by *H. Bethge* and *H. Höche*, both Halle, GDR; low energy electron microscopy by *E. G. Bauer*, Clausthal, FRG; scanning tunnel microscopy by *R. M. Feenstra*, Yorktown Heights, USA, and *R. J. Behm*, München, FRG) which reveal many details and beautiful images. The diffraction techniques (low energy electron diffraction by *M. G. Lagally*, Madison, USA, and *W. Moritz*, München, FRG; helium atom scattering by *J. P. Toennies*, Göttingen, FRG; X-ray scattering by *E. Vlieg*, Amsterdam, Netherlands) are complementary due to their ability to supply quantitative information.

If the existence of steps, their shape, density, and distribution on a surface is known, it is of interest, which kind of properties may be influenced or even determined by those steps. Some theoretical reviews on total energy calculations for semiconductors (*J. Chadi*, Palo Alto, USA) and for metals (*P. M. Marcus*, Yorktown Heights, USA) showed atom arrangements at steps to be quite different from ideal lattice sites. There are now a wide variety of well established and quantitatively measured properties due to the presence of steps. Some properties are inherently coupled with steps, like crystal growth, which was discussed experimentally (*E. Bauser*, Stuttgart, FRG, and *H. Höche*, Halle, GDR) and theoretically with quite different methods and aspects (*E. V. Albano*, Mainz, FRG, and *G. Stoyanov*, Sofia, Bulgaria). Of course, many studies on adsorption, desorption and reaction clearly show the quite different effects of steps (*K. Wandelt*, Bonn, FRG; *C. Benndorf*, Hamburg, FRG, and *G. A. Somorjai*, Berkeley, USA). Over twenty posters exhibited many details of important new developments.

All these results demonstrated, that atomic steps are not just unknown or disliked disturbances of an otherwise well-defined experiment. Including steps in all considerations brings the investigated surface closer to reality and to reproducibility. It is clear that the experiments on the best, defect free surfaces are better described and discussed when defects like steps are included. This extension is needed, since many properties are strongly influenced, e.g. for adsorption, the edge sites have a different binding energy and different vibrational modes. Due to this knowledge, many high index faces are under investigation, since they provide two or more very different surface sites. Although these faces are not yet known in as much detail as the low index phases, both microscopy and diffraction provide an increasing amount of detail. Finally a new field of properties becomes available by the inclusion of step properties. Any variation of the shape of a surface during the experiment requires the formation or variation of steps. There was an interesting discussion on the probability of crossing a step during surface diffusion. The roughening of a step during growth, due to heating is a more and more tractable phenomenon. The behavior of adsorbates at steps may change drastically and a study of this may lead to a detailed description of catalysis. Some adsorbates may even initiate a rearrangement of step atoms so that the surface forms new facets. Therefore the stability of surfaces is now to be studied taking into account processes at steps.

Of course, steps are not the only present and only important defects on surfaces. They are, however, the best investigated, and are therefore the model for all other defects. The workshop provided not just the state of the art information, but helped to combine the available information to form new ideas.

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