Chapter 6

Helium Atom Scattering Measurements on the $\alpha - Ga(010)$ Surface

Helium Atom Scattering Machine

Fig.1, *Fig.2* and *Table 1* are showing the schematic and pumping diagram of the HAS machine. The machine consists of 8 independent vacuum chambers: Nozzle chamber, chopper chamber, differential pumping stage, main chamber, three differential pumping stages and a detector chamber. The source and chopper chambers are pumped by diffusion pumps, other chambers are pumped by turbo molecular pumps. The beam spots on the chopper disk and on the sample surface are about 0.4 mm and 1mm respectively. The angular resolution (2Θ) is about 0.13°. The flight length between the chopper disc and the detector is about 1512 mm. The sum of the incident angle and scattering angle is fixed at 90°. Using the single chopper, the beam is chopped into 10 μs pulses (open time) at 666 Hz for time-of-flight measurements.

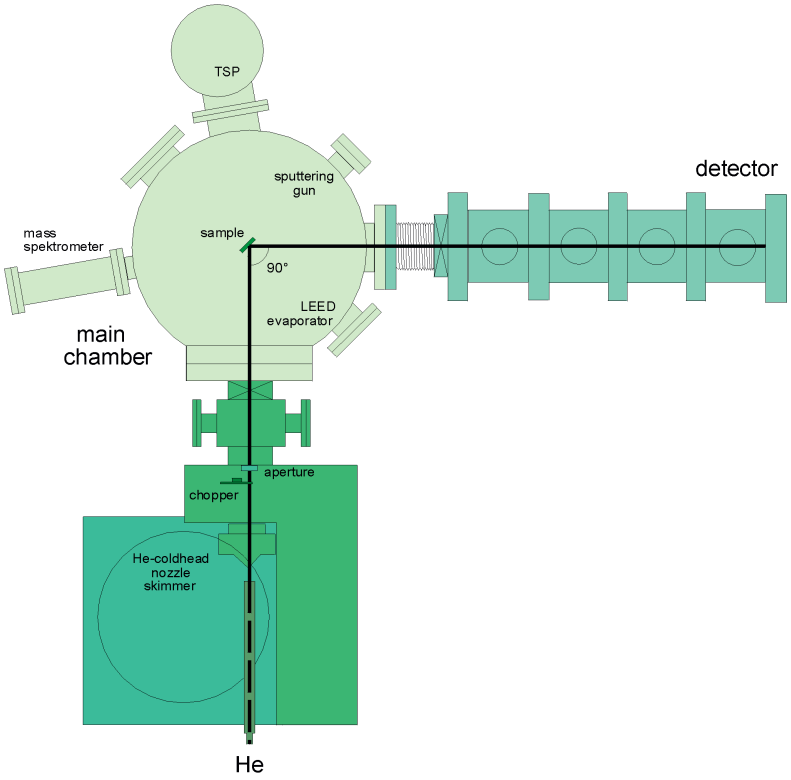

Fig.1

He scattering machine.

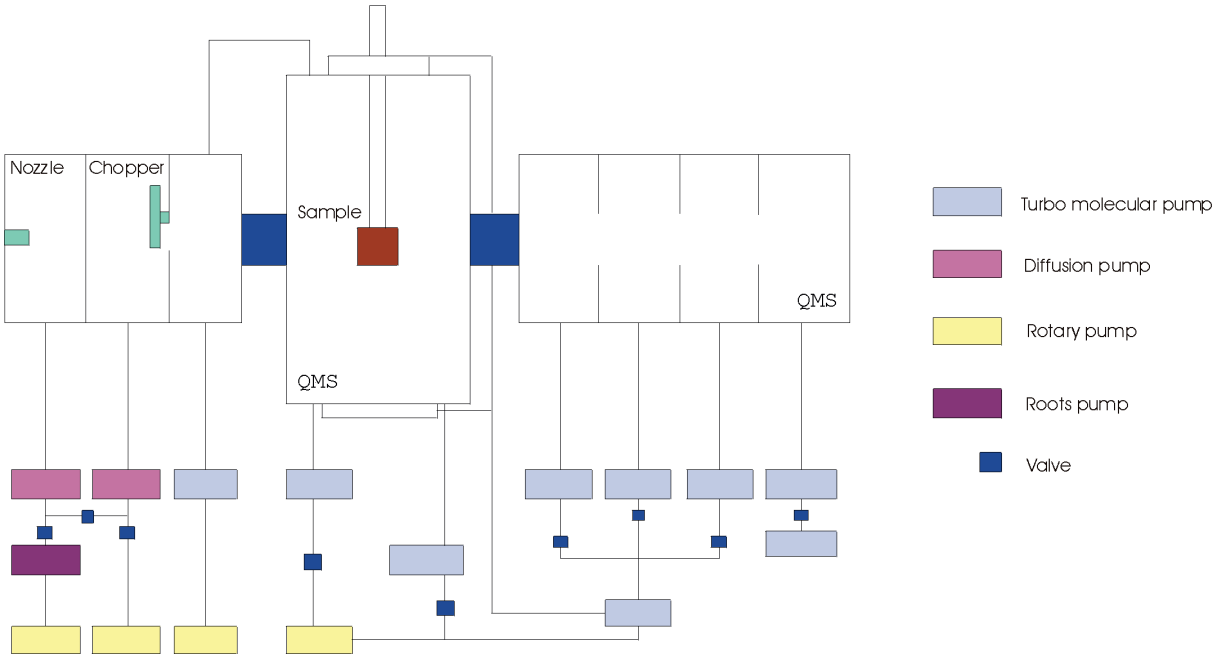

Fig.2

Schematic diagram of the Helium atom scattering machine.

Table1

Pumping system

Pump	Pumping speed	chamber
Big diffusion pump	5200 l/s	Nozzle chamber
Roots pump	270 m^3 /h	Nozzle chamber
Rotary pump	38 m^3 /h	Nozzle chamber
Small diffusion pump	2000 l/s	Chopper chamber
Rotary pump	18 m^3 /h	Chopper chamber
Turbo molecular pump	180 l/s	First differential pumping stage
Rotary pump	4 m^3 /h	First differential pumping stage
Turbo molecular pump 1	450 l/s	Main chamber
Turbo molecular pump 2	56 l/s	Main chamber
Rotary pump	4 m^3 /h	Main chamber
Turbo molecular pump 1	60 l/s	Differential pumping stage
Turbo molecular pump 2	170 l/s	Differential pumping stage
Turbo molecular pump 3	210 l/s	Differential pumping stage
Turbo molecular pump 4	33 l/s	Differential pumping stage
Turbo molecular pump 1	230 l/s	Detector chamber
Turbo molecular pump 2	60 l/s	Detector chamber

Helium Atom Scattering Experiment

Our measurements have been performed with a helium scattering apparatus which allows elastic and inelastic (time of flight) measurements. A nearly monochromatic ($\Delta v/v = 1\%$) low energy He beam is produced by expanding the high pressure (30 bar) He gas through a nozzle which was kept at 100 K temperature. This gives a beam energy of E = 23 meV; the angular divergence of the beam is below 0.05°. The base pressure of the target (main) chamber is $5x10^{-11}$ mbar which allows the Ga surface to stay clean for 15 – 20 hours. LEED measurements were taken with a four-grid LEED optics (Omicron) in the main chamber. The identification of all ordered structures was made with LEED. The α-Ga (010) surface was cleaned by several sputtering cycles with 1keV Ar^+ gas at a sample temperature close to 0°C which was enough to remove the native oxygen layer [1,2] which is due to exposure to the atmosphere before transfer into the UHV system. Once a clean surface had been obtained, ten minutes of sputtering around 0°C prior to measurements were sufficient to assure the cleanliness of the surface. Throughout the measurement period the Ga sample had to be cooled by liquid Nitrogen to avoid the melting of the crystal and subsequent contamination of the UHV system.

The cleanliness of the $\alpha - Ga(010)$ surface was checked by LEED and by polar elastic He scans. Between 235 K and 303 K α-Ga shows the (1x1) diffraction pattern. The diffraction pattern is nearly cubic and every second spot in [100] direction is missing. This is due to the glide-symmetry of the bulk in this direction. Therefore the glide symmetry persists at the surface. The more sensitive elastic He scattering results in the sharp diffraction pattern *(Fig.3a)* and is in agreement with the LEED data. When the sample is cooled below 235 K, a reversible phase transition can be observed. The LEED diffraction pattern at 100 K shows a c(2x2) structure. The previously missing spots are now visible which is compatible with a loss of glide-plane symmetry. An investigation with a more sensitive SPA-LEED technique showed additional spots, which confirms that the structure is $\left(2\sqrt{2}x\sqrt{2}\right)R45°$. The intensity of these spots is small and with a standard LEED they are not observable [2]. The additional shoulder next to the diffraction maximum *(Fig3b)* might be attributed to further structural details. It can not be explained with a spot splitting as a result of the long range periodicity of the low temperature Ga phase because the splitting itself is not along this direction in k-space.

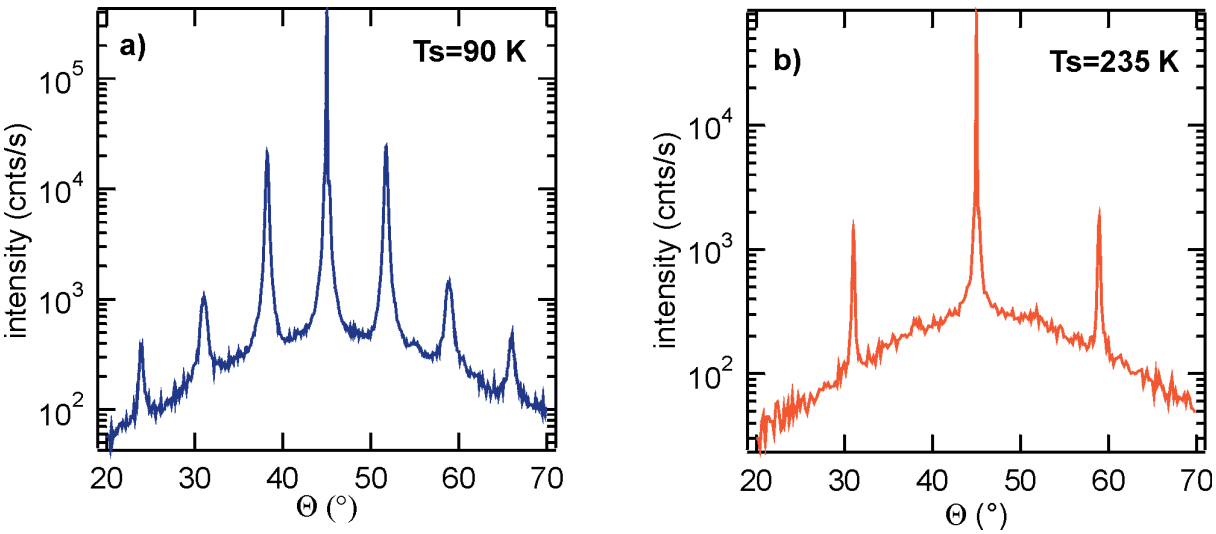

Fig 3a

Angular distribution of the scattered He intensity along the [110] direction on the Ga surface measuresd at (a) 90 K and (b) 235 K.

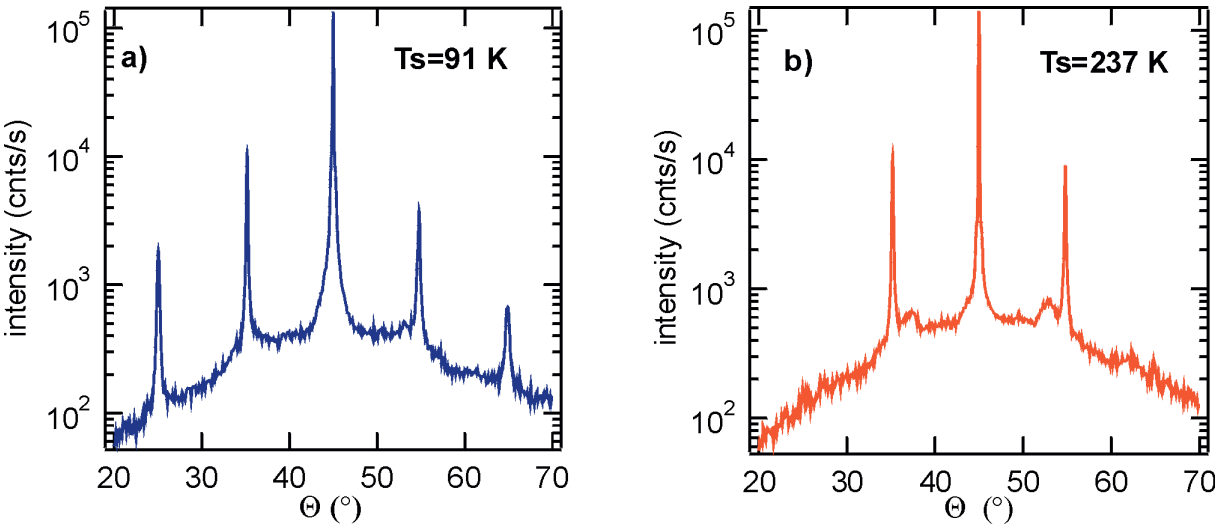

Fig 3b

Angular distribution of the scattered He intensity along the [100] direction on the Ga surface measuresd at (a) 91 K and (b) 237 K.

Surface phonons

Inelastic scattering experiments were used to investigate the surface phonon dispersion curves above and below the phase transition. For the experiment two kinds of choppers were used: A standard single chopper and a pseudo-random chopper. For the use of optimal performance in accordance with the maximum achievable rotational speed, a sequence with 511 elements in the pseudo-random chopper was chosen and repeated twice, resulting in a medium slit width of 0.516 mm. The normal chopper is arranged on a larger diameter on the same chopper disk and can therefore easily be switched to. The intensity by using the random chopper is much higher than those with the normal chopper.

The surface phonon dispersion curves above and below the phase transition measured with the single chopper are shown in *Fig.4a/b*, and with the random chopper in *Fig.5a/b*. The solid lines are a guide to the eye. The reduction of the Brillouin zone is in agreement with the structural transition discussed above.

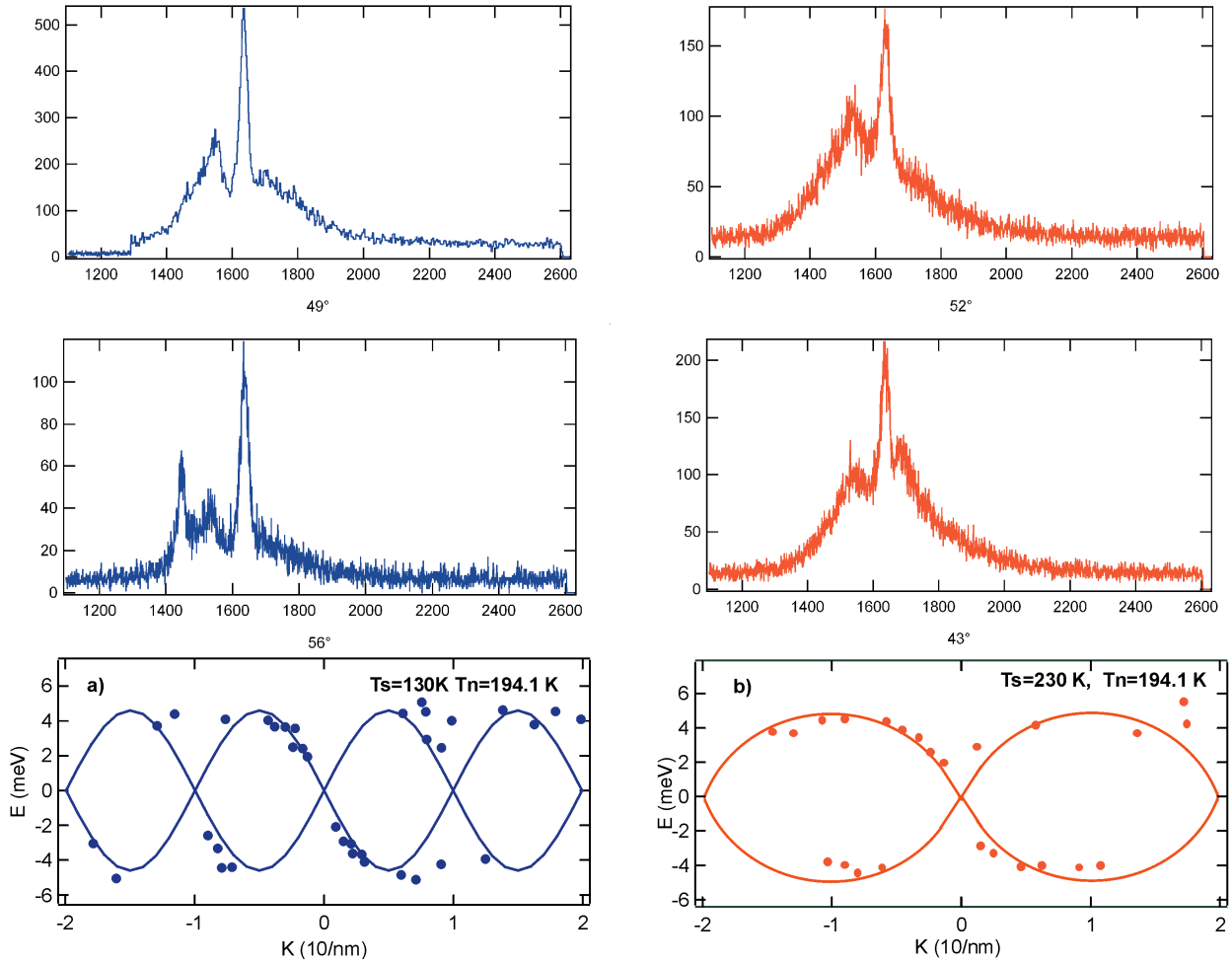

Fig.4

Some representative time-of-flight spectra measured with a normal chopper for low temperature phase (blue) and room temperature phase (red). The unit of the horizontal scale is ms, vertical scale displays counts per measuring time interval.

The surface phonon dispersion curves below (a) and above (b) the phase transition measured with the single chopper for the [110] direction.

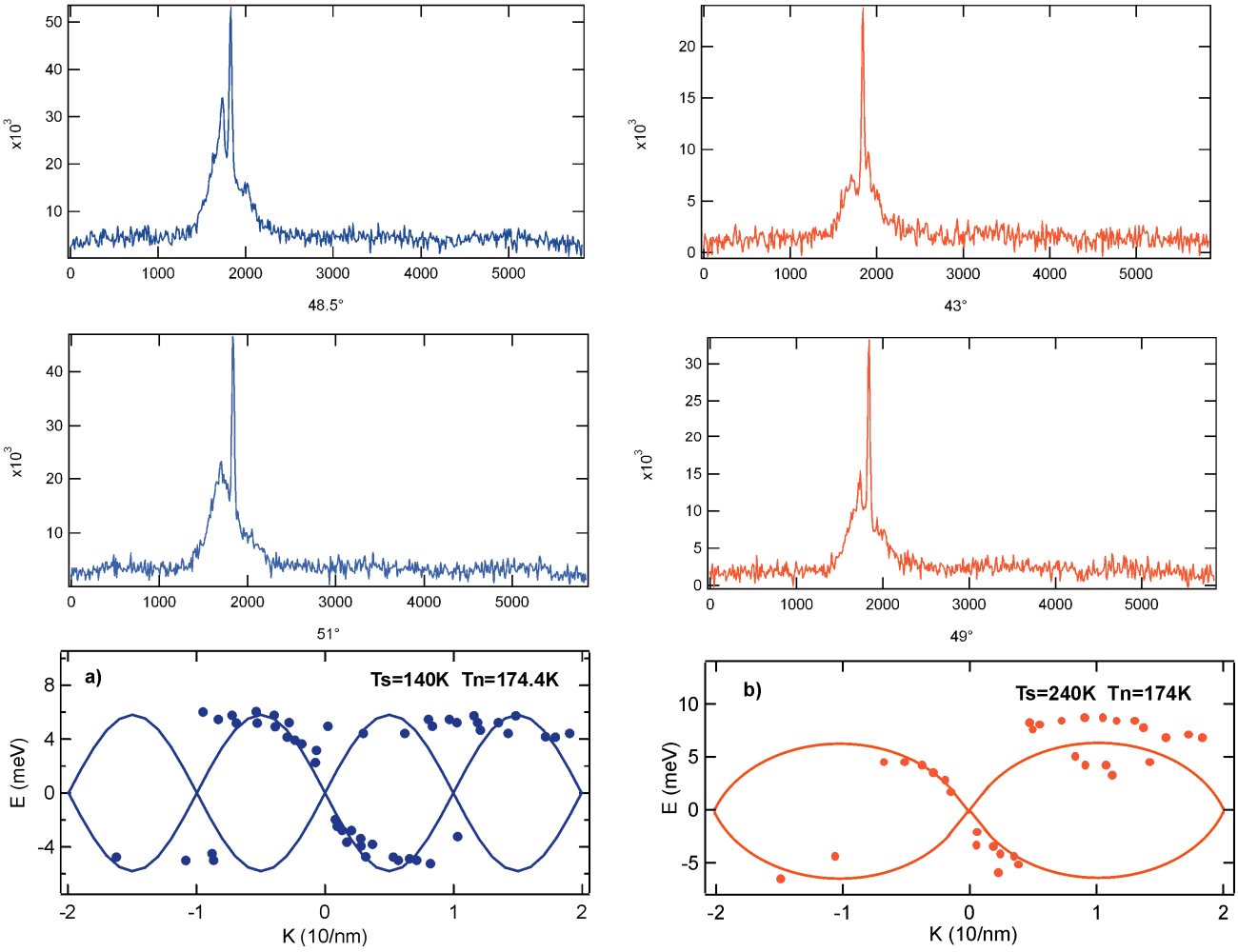

Fig.5

Some representative time-of-flight spectra measured with a random chopper for low temperature phase (blue) and room temperature phase (red). The unit of the horizontal scale is ms, vertical scale displays counts per measuring time interval.

The surface phonon dispersion curves below (a) and above (b) the phase transition measured with random chopper for the [110] direction.

The highest phonon energy measured with the normal chopper above and below the phase transition amounts to 5 meV. The highest phonon energy measured with the random chopper in the low temperature phase amounts to 6 meV, while in the room temperature phase 5 meV and 9 meV have been measured. Here the data shows a distribution between two limits, most likely due to the fact that the chopper openings are random, but repeating. So actually the slit distribution is pseudorandom resulting in additional peaks in phonon spectra. In principle a change of the chopper rotation frequency would shift these peaks.

The inelastic HAS experiment shows the change in periodicity in the phonon dispersion spectra in accordance with the elastic measurements. Phonon energy level limits for the Ga(010) surface have been estimated within a Debye model evaluating data from photoemission spectroscopy [1]. From the temperature dependence of the linewidth of the surface state a value for the Debye cutoff frequency of 28 meV was determined. This value still includes Auger decay and defect scattering and therefore is a too crude estimate for a direct comparison with the results measured here. The value measured by photoemission spectroscopy includes contributions from the bulk since photoemission spectroscopy is not exclusively surface sensitive and even surface electrons have a substantial interaction with bulk phonons. But a recent theoretical investigation for the Cu (111) and the Ag (111) surfaces revealed that the dominant contribution to the linewidth comes from the Rayleigh mode [3]. Therefore the value obtained by photoemission spectroscopy displays in principle the linewidth for the surface but can not be compared with the results from HAS for the above mentioned reasons.

Conclusion

For the first time the α-Ga (010) surface was investigated by helium atom scattering. Elastic scattering confirmed a second order phase transition from a (1x1) structure to a $\left(2\sqrt{2}x\sqrt{2}\right)R45°$ structure at 235 K. With time-of-flight measurements the phonon dispersion was determined above and below the phase transition. The change of periodicity in the dispersion is in accordance with the elastic scattering measurements.

References

[1] Ph. Hofmann, Y.Q. Cai, Ch. Grütter, J.H. Bilgram, PRL **81** (1998) 1670.

[2] Ph. Hofmann, Report about the SPA-LEED data taken in Trieste (not published).

[3] A. Eiguren, B. Hellsing, F. Reinert, G. Nicolay, E.V. Chulkov, V.M. Silkin, S. Hüfner, P.M. Echenique, PRL **88**, 066805 (2002).