ESRF	**Experiment title:** Anisotropic molecular vibrations in solid hydrogen determined by angle-dispersive single crystal X-ray diffraction.	**Experiment number**: HS-914
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Report:

The aim of this experiment was twofold: on one hand it served as a test example to explore the potential of the newly installed high-pressure-single crystal facility on ID30 (developed and installed by Larry Finger, Stefan Carlson and Martin Kunz) with a most challenging sample (solid hydrogen crystal). On the other hand it was foreseen to contribute to solve some open questions on the high-pressure behavior of solid hydrogen.

High-pressure single crystal set-up using a one-circle diffractometer and the FastScan image-plate reader: Our experiment allowed to demonstrate that the system is sensitive enough to record diffraction spots from weak scatterers such as H_2 even through a diamond anvil cell. We managed to write and adapt software allowing us to index the diffraction spots and predict positions of yet unrecorded spots. By this way, we were able to see diffracted intensity up to the maximal pressure of 30 GPa. At the highest pressure, however, the lack of a He-pressure medium caused the crystal to crack which lead to badly deformed or even split peaks. This made it impossible to extract any useful intensities at these pressures. Experiments with various diamond anvil cells showed that for a successful single crystal experiment with an area detector, it is essential that the cell contains no backing disks, but rather an open cone. This to avoid contaminant reflections from boron or beryllium, which make an automated peak search impossible and a manual peak search very tedious and difficult.

Anisotropic displacement parameters of H_2 *as a function of pressure:* This part of the experiment was not quite as successful. Despite many attempts to interpret the extracted intensities in terms of anisotropic displacement parameters, we did not manage to extract physically reasonable displacement parameters out of our intensities. The reason for this is suspected in primary extinction of the incoming X-ray beam at the front-diamond. The diffraction of the primary beam at the front diamond decreases the incoming intensity by a considerable amount. This affects the measured intensity in a significant way. It turns out that it is impossible to correct for this effect *a posteriori*, mainly due to the impossibility to predict which of the sample reflections are affected and by how much. This prevents us from using the corrected intensities to extract anisotropic displacement parameters. A possible solution for this problem is to perform the experiment at two different wavelengths. Differences in the relative intensities would thus uncover extinction-affected reflections and thus enable a correction. This procedure is likely to be useful for any single-crystal experiment through a diamond anvil cell using an area detector.