Phase Determination of the Forbidden Reflection 222 in Germanium Using UMWEG-99

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The θ-ψ-scan of the "almost forbidden" reflection 222 of germanium (upper diagram in Fig. 1, lower in Fig. 2) was performed with λ = 1.1851 Å on the Huber four-circle diffractometer at beamline D3 at HASYLAB. For each step in ψ the integrated intensity of a θ-scan was collected with the step-widths Δψ = 0 .002°. The germanium crystal used for the experiment was ground to a sphere in a sphere mill. The surface roughness caused by the mechanical treatment was removed by chemical etching. In this way an ideal crystal sphere with a radius of R = 65 µm was obtained. For comparison with experimental multiple diffraction patterns in Umweg-99 [1], [3] the intensities integrated over θ are considered by [2]

$$I_{s_1}(\psi_j)_{event} = \{I_{prim} - I_{Aufh}(\psi_j)\} + I_{Umweg}(\psi_j) + 2 \cdot \sqrt{\{I_{prim} - I_{Aufh}(\psi_j)\} \cdot I_{Umweg}(\psi_j)} \cdot \cos\varphi(\psi_j),$$

with the phase difference

$$\varphi(\psi_j) = \varphi_{op} + \varphi_{coop} + \varphi_s - \varphi_{prim}.$$

Because of the centrosymmetric structure of germanium, the triplet phase $\varphi_{op} + \varphi_{coop} - \varphi_{prim}$ is 0 or π. The scattering phase-shift φ_s varies from 0 to π during the passage of reciprocal lattice point from inside to outside the Ewald-Sphere, the Bragg condition value being π/2.

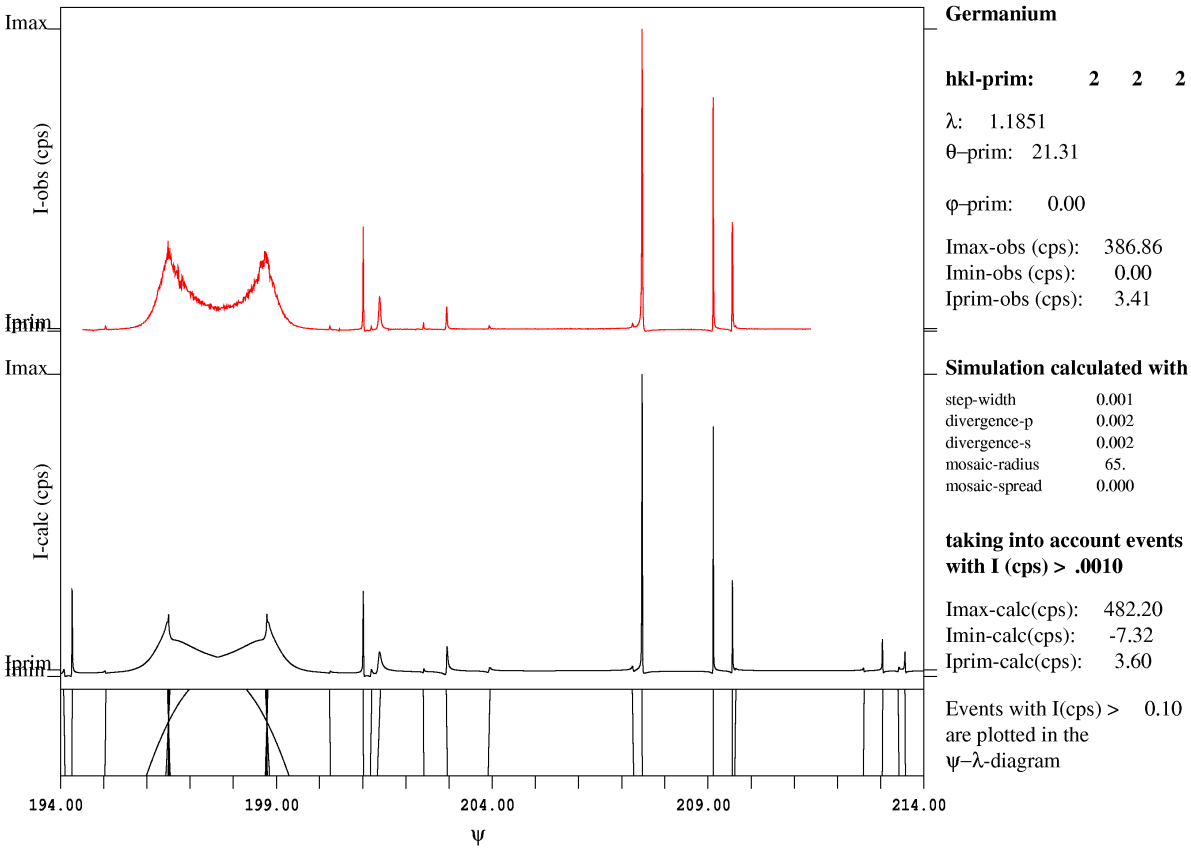

Figure 1: Output of Umweg-99 for the measured (on top) multiple diffraction pattern of the 222 reflection of germanium. Comparison with the by Umweg-99 simulated profile (below), $\varphi_{222} = 0°$.

The application of Umweg-99 to the measured multiple diffraction pattern of the 222 reflection of germanium in the region of ψ = 194 to 214° is shown in Fig. 1. A more detailed impression is gained by an opening from ψ = 206.5 to 210.5° in Fig. 2, where the high intensities are cut at a low level. The simulated scan in (b), calculated with φ_{222} = 0° according to the origin of the unit cell at 1/8 1/8 1/8, fits excellent to the measured one in (a). This is an absolute contrast to the simulation in (c), which was carried out by the use of the phase for the primary reflection φ_{222} = 180°.

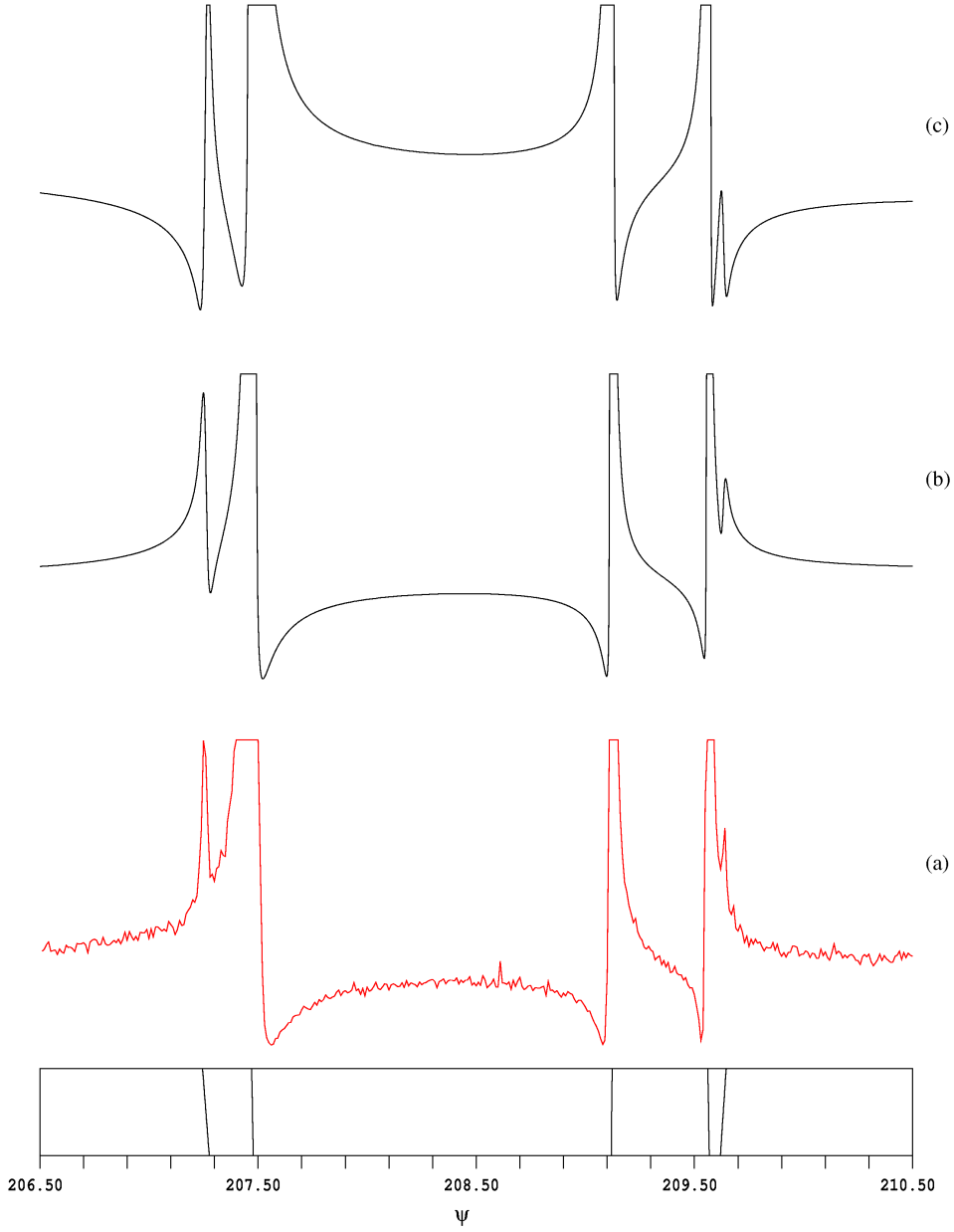

Figure 2: Multiple diffraction pattern of the 222 reflection of germanium. (a) Measured with λ = 1.1851 Å. (b) Simulated with Umweg-99, φ_{222} = 0°. (c) Simulated with Umweg-99, φ_{222} = 180°.

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References

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[3] E. Rossmanith, A. Hupe, H.-G. Krane, H. Schmidt, HASYLAB-Jahresbericht 1999