

# Evaluation of the Structure of Amorphous Tungsten Oxide $\text{W}_{28}\text{O}_{72}$ by the Combination of Electron-, X-Ray- and Neutron-Diffraction (Three-Beam Experiment)

Jürgen Ankele<sup>a</sup>, Joachim Mayer<sup>b</sup>, Peter Lamparter<sup>c</sup>, and Siegfried Steeb<sup>c</sup>

<sup>a</sup> Alcatel SEL AG, Lorenzstraße 10, D-70435 Stuttgart, Germany

<sup>b</sup> Rheinisch-Westfälische Technische Hochschule Aachen, Gemeinschaftslabor für Elektronenmikroskopie, Ahornstraße 55, D-52074 Aachen, Germany

<sup>c</sup> Max-Planck-Institut für Metallforschung, Heisenbergstraße 3, D-70569 Stuttgart, Germany

Reprint requests to Dr. P. L.; Fax: +49 (0)711 689-3312; E-mail: Lamparter@mf.mpg.de

Z. Naturforsch. **61a**, 189 – 196 (2006); received December 20, 2005

From the combination of quantitative electron-diffraction data with X-ray- and neutron-diffraction data (so-called three-beam experiment) the partial structure factors and pair correlation functions of amorphous sputter deposited  $\text{W}_{28}\text{O}_{72}$  were determined. On the basis of the experimental atomic distances and coordination numbers, and by comparison with crystalline  $\text{WO}_3$ , a structural model was developed, which consists of twisted  $\text{WO}_6$  octahedra. Reverse Monte Carlo simulation in accordance with the experimental data was performed to verify the results.

*Key words:* Amorphous Tungsten Oxide; Diffraction; RMC Simulation.