# Simulation of amorphous structures for comparison with images of aged FeCr samples

C. Kreyenschulte and H. Kohl

Physikalisches Institut, Interdisziplinäres Centrum für Elektronenmikroskopie und Mikroanalyse (ICEM)
Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster

Carsten.Kreyenschulte@uni-muenster.de
Keywords: EFTEM, elemental maps, simulation, diffractograms

Extending our previous work on determining the two-particle-structure factor from inelastic diffractograms, we now compare simulations of amorphous structures with experimental data.

The method used to acquire the experimental data has been described in previous publications [1,2,3,4,5]. The Fourier transform of an elemental map $I_{CCD}(u)$ consists of several factors. The one of interest for us is proportional to the two-particle-structure factor $S_{aa}(u)$. The other terms are the modulation-transfer function $MTF(u)$ describing the CCD-camera characteristics. It is usually supplied by the camera manufacturer. The drift function $D(u)$ describing the sample drift during acquisition can be calculated from the image itself. The inelastic transfer function $ITF(u)$ describes the microscope's characteristics and the scattering process in dipole approximation. It can be calculated theoretically. The additional term B(u) describes the white noise of the image.

$$\left|I_{CCD}(u)\right|^2 = MTF(u)^2 \cdot D(u)^2 \cdot ITF(u)^2 \cdot S_{aa}(u) + B(u).$$

These diffractograms of the elemental maps were treated to compensate for the influence of these factors. The result is proportional to the two-particle-structure factor.

To analyze the two-particle-structure factor further, we started simulating amorphous structures. For simplicity we use arbitrarily distributed spheres. The radii of the spheres are described as a Gaussian distribution.

For our experiments we used an alloy consisting of 45 at% iron and 55 at% chromium, aged for two weeks at 550°C. The elemental maps were taken at 595eV energy loss for chromium and at 725 eV for iron (Figures 1 and 2). After calculating the two-particle-structure factors we try to fit the simulation parameters to achieve a good agreement with the experimental data (Figure 3).

Our further work now concentrates on identifying the remaining influences of image noise and sample defect structure as well as improvements in the simulation code.

1. H. Kohl, H. Rose, Adv. Electron El. Phys. **65** (1985), 173-227.
2. R. Knippelmeyer and H. Kohl, J. Microscopy **194** (1999), 30-41.
3. A. Thesing, PhD Thesis, University of Münster.
4. C. Kreyenschulte and H. Kohl, Microsc Microanal **13** Suppl 3 (2007), 284-285.
5. C. Kreyenschulte and H. Kohl, EMC 2008, Vol. 1: Instrumentation and Methods, Springer (2008), 401-402.

G. Kothleitner, M. Leisch (Eds.): MC2009, Vol. 1: Instrumentation and Methodology,
DOI: 10.3217/978-3-85125-062-6-073, © Verlag der TU Graz 2009

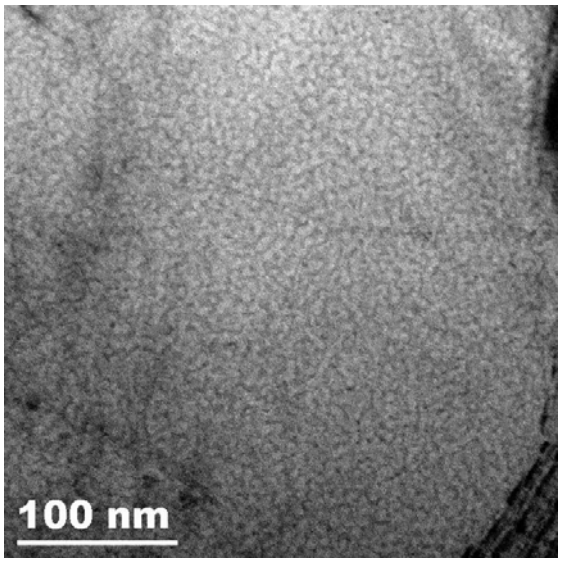


**Figure 1.** Elemental map of chromium, taken at 595 eV.

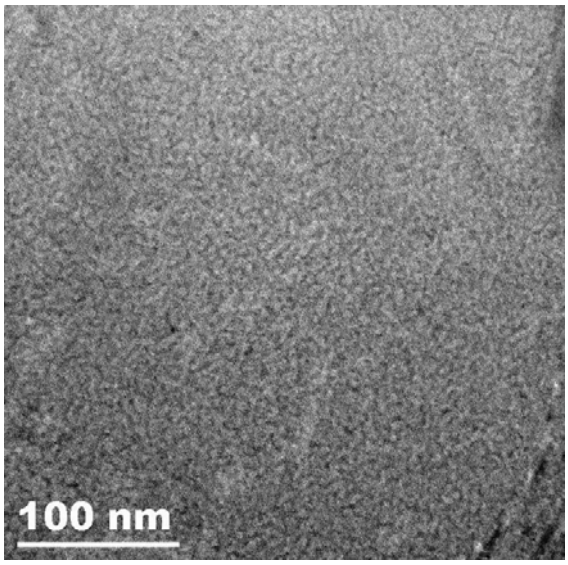


**Figure 2.** Elemental map of iron taken at 725 eV.

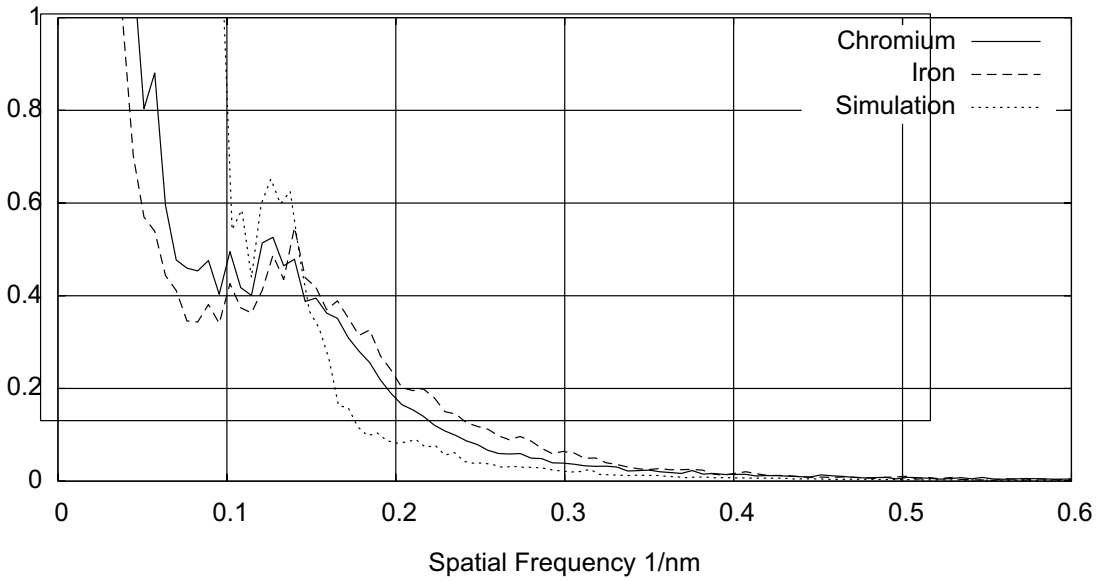


**Figure 3.** Structure factors of iron and chromium compared to a simulated structure with a mean sphere radius of 6.5 nm.

G. Kothleitner, M. Leisch (Eds.): MC2009, Vol. 1: Instrumentation and Methodology,
DOI: 10.3217/978-3-85125-062-6-073, © Verlag der TU Graz 2009