Atomic-level elastic strain measurement of amorphous materials by quantification of local selected area electron diffraction patterns

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Metallic glasses have been promising materials for application as structural materials. Therefore, intense research has been carried out to understand their mechanical properties and the underlying physical phenomena [1]. An important aspect of this research is measuring the response of metallic glasses to external and/or internal stresses and the resulting atomic displacements. These atomic level strains can be measured by quantification of the peak shifts in synchrotron diffraction experiments as demonstrated by Poulsen et. al. [2].

Here, we present a novel TEM method for measuring the atomic level strains on a local scale by means of electron diffraction. A series of selected area electron diffraction (SAD) patterns of amorphous TiAl tensile test samples are recorded in a CM200 electron microscope equipped with a Gatan Orion CCD camera. External stress is applied in-situ and the evolution of the 2D strain tensor is calculated from the distortion of the characteristic amorphous diffraction halo. The full evaluation is carried out automatically by a plugin written for the Digital Micrograph™ platform: The peak maxima positions are extracted with sub-pixel accuracy from azimuthal integrated sectors of 1° (cf. Fig.1(a)). This is achieved by a non-linear least squares fit using a pseudo-Voigt model function (cf. Fig.1(b)). By fitting an ellipse to the maxima positions also the center is determined with sub-pixel accuracy. By iteration the data is refined and the polar form of the maxima positions is obtained. Using an unstrained SAD pattern as reference, the 2D strain tensor can be calculated from the difference of the peak maxima positions. By fitting the polar form of the strain tensor finally the principal strain magnitude and direction can be obtained relative to the SAD patterns coordinate system (cf. Fig. 2).

Simulated diffraction patterns with known parameters and different levels of noise are used to check the strain accuracy of the method. The relative error is calculated with respect to the known input parameters. The method has an accuracy of about $1x10^{-4}$ in determination of the parameters, the relative error in principal stress is below 3% even at principal strain below 0.5% (cf. Fig. 3).

In addition to measure the atomic-level strain response to an applied external stress the method allows also to map the strains on a local scale, limited in principle only by selected aperture size and intensity fluctuations of the diffraction data for small sampling volumes. An example for such mapping capabilities is given in Fig. 4, where the strain distribution over the width of a strained specimen is given. In this case the strain distribution is non-uniform and varies between 1.3% at center and 1.35% at edge regions.

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[2] H.F. Poulsen, J. a. Wert, J. Neuefeind, V. Honkimäki, M. Daymond, Measuring strain distributions in amorphous materials, Nat. Mater. 4 (2005) 33–36. doi:10.1038/nmat1266.

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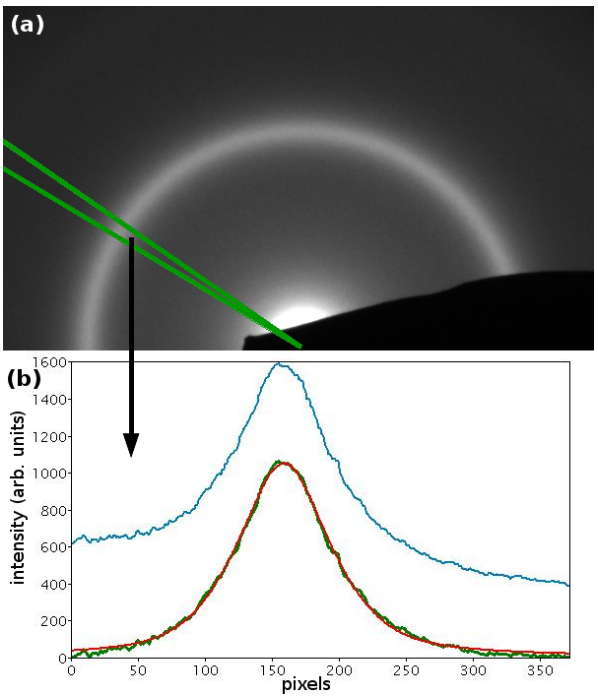

Figure 1: Determination of the peak maxima positions: (a) The diffraction pattern is divided into sectors with fixed size (green lines, e.g. 1°). All sectors are integrated azimuthally and constrained by a user given mask to obtain the line profiles. (b) A linear background is subtracted from the profiles and the peak fitted by a pseudo-Voigt model function.

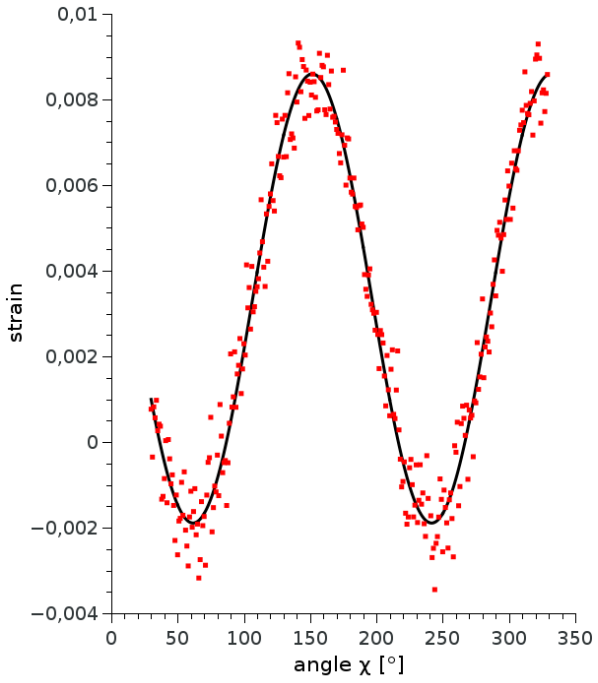

Figure 2: Calculation of the principal strain: The 2D strain tensor is obtained by calculating the angular dependent strain for each sector relative to a reference and fitting these data points. By calculation of the eigenvalues of the 2D tensor the principal strains are obtained.

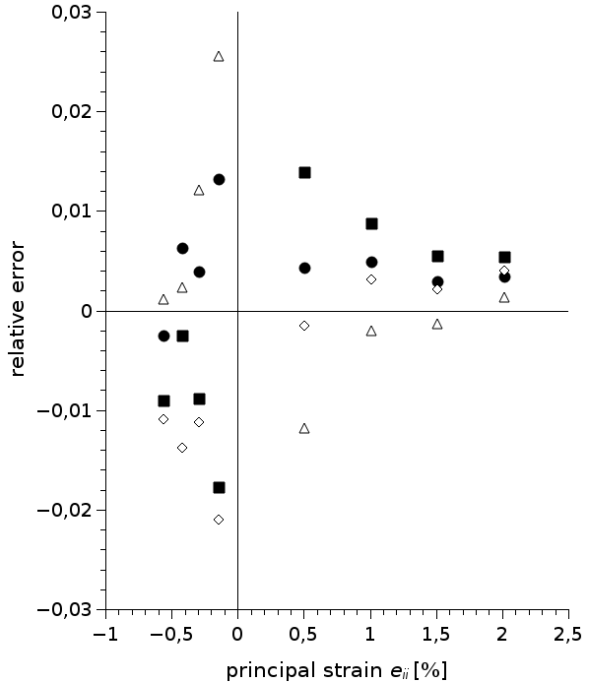

Figure 3: Error evaluation: The accuracy of the fit is checked by artificial diffraction patterns with known distortions. Open and closed symbols refer to simulated data with different additional noise levels. At low strains the error is below 3%. For larger strains the rellative error decreases.

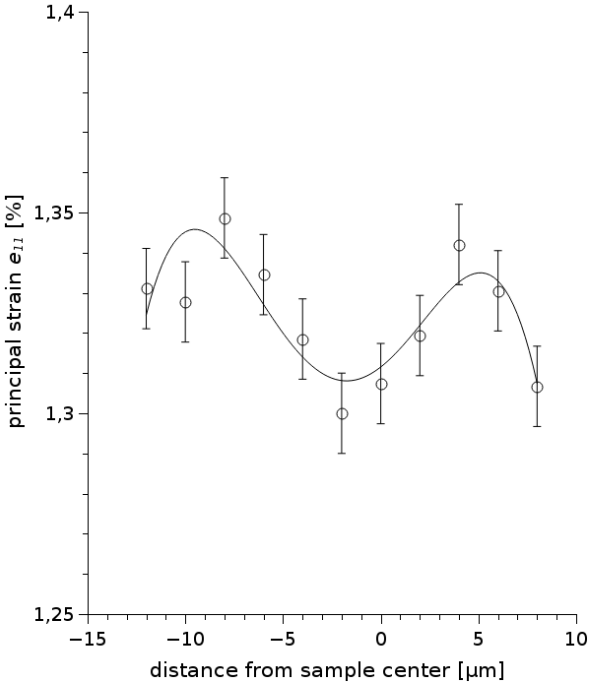

Figure 4: Strain mapping: By recording a series of diffraction patterns over the width of a strained specimen the local changes in strain behaviour are observed. A polynomial fit is included to guide the eye.