DISLOCATION DENSITY, CHARACTER AND BURGERS VECTOR TYPES IN CUBIC AND HEXAGONAL CLOSE PACKED CRYSTALS DETERMINED TOGETHER WITH OTHER DEFECTS BY DIFFRACTION LINE PROFILE ANALYSIS USING TIME OF FLIGHT NEUTRON DIFFRACTION MEASUREMENTS

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Diffraction line profile analysis (DLPA) is a powerful tool for characterization of the microstructure of crystalline materials [1,2]. In the last decade considerable effort has been made to develop DLPA procedures that can determine the parameters of the microstructure by fitting whole diffraction patterns [1,3]. For the work presented here the extended Convolutional Multiple Whole Profile (eCMWP) DLPA software has been used [3]. The theoretical profile functions used by the eCMWP software are calculated as the convolution of the theoretical size and strain (dislocation) and planar fault profiles and measured instrumental profiles [3,4]. These theoretical profile functions, which have as parameters the characteristics of the microstructure, are fitted to the measured data by a non-linear least-squares algorithm and thus the parameters of the microstructure are determined.

Until now, the DLPA method has been used mostly with X-ray diffraction patters. There is interest in using Time-of-Flight (TOF) neutron diffraction data for DLPA due to the high penetration of neutrons and because TOF diffraction records many peaks simultaneously with collinear diffraction vectors [5]. TOF neutron instruments are capable of collecting diffraction data with sufficient statistics and resolution to make the DLPA technique possible. However, in case of time-of-flight (TOF) neutron diffraction measurements there is a non-negligible asymmetric instrumental broadening effect. The eCMWP software convolutes the measured instrumental diffraction peaks directly with the theoretical profile functions to get the final pattern which is fitted to the measured data, this way making it possible to analyze TOF neutron diffraction data.

The data for the presented DLPA applications have been collected at the Los Alamos Neutron Science Center (LANSCE) using the Spectrometer for Materials Research at Temperature and Stress (SMARTS) and the Neutron Powder Diffractometer (NPDF) TOF neutron diffraction instruments. In-situ measurements have been done during tensile deformation of stainless steel and TWIP steel samples on the SMARTS instrument and using DLPA the dislocation and planar fault densities have been determined as a function of strain. Zr alloy samples removed from service in a nuclear power reactor were investigated using the NPDF instrument, to determine the microstructural changes caused by heavy neutron irradiation inside nuclear reactors. It will be shown, that several years spent inside a nuclear reactor causes a dramatic increase in the <a> Burgers vector type dislocation density in Zr and the arrangement of the dislocation structure changes fundamentally too. These investigations are of great technological interest as Zr alloys are used as structural material in nuclear reactors.

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