MS36-05 **High pressure research using dynamic compression at the European XFEL** Thomas Tschentscher,[a] Thomas E. Cowan,[b] Hanns-Peter Liermann,[c] *[a]European XFEL GmbH, 22607 Hamburg, Germany, [b]Helmholtz-Zentrum Dresden Rossendorf, 01328 Dresden, Germany, [c]DESY, 22607 Hamburg, Germany*
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The integration of a high energy nanosecond pulse duration laser system in the High Energy Density (HED) instrument of the European XFEL [1] will enable studying atomic structure of materials at extreme pressures and densities. So-called ramp compression [2] using shaped nanosecond laser pulses will allow to generate states of pressure exceeding current limitations of static compression avoiding at the same time steep temperature rise following hugoniot curves. The development and implementation at European XFEL of the required optical laser system with pulse energies in the range beyond 100 J, temporal shaped nanosecond pulses and repetition rates of 0.1 to 10 Hz was recently proposed by an international consortium. Probing of the dynamic, optical laser generated high pressure states will be performed by using high brilliance ultrashort pulse hard x-ray free electron laser (FEL) radiation. In the regime 5 to 25 keV it will be possible to use diffraction, spectroscopy or imaging techniques for investigations of the geometric and electronic structure. The intensity and overall time resolution will enable to perform time-resolved analysis of the evolution of the dynamically compressed systems. Furthermore the high brilliance and coherence of the FEL radiation shall be employed for higher measurement accuracy using spatially resolving techniques avoiding integration over sample volumes of varying excitation and thermo-dynamical properties. Such techniques would become extremely important in case of non-planar and microscopic sample excitation using focused optical laser pulses.

[1] for detailed information about European XFEL see *www.xfel.eu*
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MS37-01 **Structure determination of intermetallics using Precession Electron Diffraction.** Louisa Meshi,[ab] Shmuel Samuha,[ab] *[a]Department of Materials Engineering, Ben-Gurion University of the Negev, Beer-Sheva, Israel, [b]Ilse Katz Institute for Nanoscience, Ben-Gurion University of the Negev, Beer-Sheva, Israel.*
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Commonly, structure solution is performed using X-ray diffraction data. However, if single crystals of studied materials are unavailable and/or the alloy contains multiple complex phases – single X-ray diffractometry can not be used and powder X-ray diffraction is powerless due to severe peak overlapping, especially if studied phases are of nano size and peak broadening occurs. In such cases, electron crystallography (EC) emerges as the only tool for structure determination. Although EC was not commonly used for determination of atom positions due to dynamical nature of electron diffraction intensities, the situation has changed when Precession Electron Diffraction (PED), which produces quasi-kinematic intensities, was invented [1]. Using PED method, structures of minerals, complex oxides and zeolites were solved by several research groups. Structures of intermetallics were not solved previously using solely electron diffraction methods. Reason for that is in the nature of intermetallic compounds. Contrarily to zeolites or complex oxides, the atomic distances and angles of intermetallics are not fixed and coordination polyhedra are usually unknown. Thus, structure solution of these compounds is harder to validate and appropriateness of EC methods for their structure solution should be addressed. Present work shows structure solution of several ternary alluminides (as an example of intermetallics) using solely electron crystallography methods. Atomic model was successfully deduced from PED data.

Presented structure solution path was chosen and variable parameters (such as exposure time and precession angle) tuned basing on solution of known cubic Al-Mg structure, then the proposed path was used for structure solution of unknown ternary alluminides.

For determination of geometry of the unit cell – Selected Area Electron Diffraction in precession mode was used. Due to the fact that all studied structures had relatively high values of lattice parameters, conventional Convergent Beam Electron Diffraction method could not be used for characterization of their symmetry. For this purpose, microdiffraction technique [2] was successfully applied. Atomic model was determined by following path: observation of PED patterns from the studied phase at different orientations; extraction of the intensities and building a dataset (we have used ELD and Triple softwares [3]); use these data as an input for direct methods utilized in SIR package [4]. We concluded that one of the most important values for evaluation of sufficiency of data (extracted from PED patterns) for structure solution is number of unique reflections. The bigger this value – the better and reliable is the solution. Other factors checked: the necessity of Lorentz correction - which proved to worsen the data; and kinematicity of PED intensities. Successful solution of new alluminide phases found in various ternary systems will be presented.

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