

MS21-P6 Comprehensive Analysis of Disorder in NaLaF₄: an Efficient Up-Conversion Phosphor

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NaLaF₄ is an efficient up-conversion phosphor [1] belonging to the family of rare earth-doped sodium lanthanide tetrafluorides where the nature of the photoactive sites can unambiguously be explained only in terms of a microscopic model of disorder [2]. X-ray and Neutron Diffuse Scattering (XDS, NDS), as *k*-space probes, provide statistically reliable data on atomic pair correlation functions and thus on deviations from the average periodic structure. Using high quality XDS and NDS datasets from the distinctive, planar diffuse scattering of NaLaF₄, we calculated the 3D-Difference Pair Distribution Function (3D-ΔPDF), identified the various types of disorder and derived an abstract model of interatomic vectors [3]. It was then possible by means of Monte Carlo (MC) simulations to build and optimize large model crystals providing a specific atomistic disorder model for NaLaF₄, whose Fourier transform gives an excellent fit to the experimental diffuse scattering. The distinct contrast displayed by the various atomic species with the two radiation types provides a better sensitivity to the different pair-wise correlations ultimately yielding more robust results.

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Keywords: photo-active materials, disorder, diffuse scattering

MS21-P7 Unraveling Two-Dimensional Polymerization Propagation from Diffuse Scattering

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A recent advance in polymer chemistry is two-dimensional polymerization [1]. This is achieved by pre-organizing trifunctional monomer molecules through crystallization followed by exposure of the crystal to intense light. This external trigger propels a thermally reversible photochemical reaction and genuine long-ranged ordered two-dimensional polymerization is accomplished.

The monomer molecules used in this study [2] crystallize in the chiral and polar space group *R*3. Polymerization occurs in the *ab*-plane of the crystal. Despite large structural changes during polymerization and depolymerization, the space group is preserved in this single-crystal-to-single-crystal transformation. Both, polymerization and depolymerization can be frozen in time by simply removing the crystal from the triggering source thus creating a disordered monomer/polymer single crystal. The highly polar solvent molecule 2-cyanopyridine is incorporated into the structure in an orientationally disordered manner. This disorder is altered by the polymerization reaction.

This contribution will address two-dimensional polymerization propagation by means of real crystal structure analysis. Three imaginable propagation models with different distributions of bonded monomer moieties are presented in Figure 1. Unlike Bragg scattering, diffuse scattering [3] is sensitive to the distribution of these bonded monomer moieties. High-resolution synchrotron measurements were done to record the diffuse scattering during the polymerization and depolymerization. Several different diffuse scattering features were observed and will be presented and qualitatively interpreted. The newly developed 3D-ΔPDF method [4] and Monte Carlo simulations will be employed to model the real structure. The combined results will reveal the type of polymerization propagation. Furthermore, additional aspects caused by the polymerization will be discussed, such as the overall change in the electric dipole momentum caused by the reorientation of the solvent molecules or the crystal quality.

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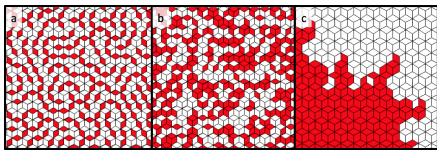


Figure 1. Schematic visualization of three imaginable propagation types. The image shows snapshots from (a) dimerization-like, (b) random-like and (c) nucleation-like polymerization propagations. Although all three models exhibit the same average structure, they have very different real structures.

Keywords: Disorder; Diffuse Scattering; PDF; Polymer

MS21-P8 Order change and phase's redistribution in single crystal of Ni-based superalloy during hard cyclic viscoplastic deformation

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The X-ray investigation of cuts and spheres of complex alloyed single crystal (SC) of Ni-based superalloy ZS-32 have been carried out for samples with identical solidification parameters prior to identical casting conditions and after different levels of hard (tension-compression) cyclic viscoplastic (HCV) deformation. The microstructure evolution of the cast samples have been studied in a plane, parallel to solidification direction, using optical microscope (Nikon Microphot-FX) and scanning electron microscope (Zeiss EVO MA-15) equipped with energy dispersive spectrometer (EDS) system for local chemical composition determine of different phases. The lattice constant and atomic occupancy have been determined use Siemens and CCD single crystal diffractometer Xcalibur with MoK-alpha-radiation. The 7000-8000 Bragg reflections have been collected in full Ewald sphere. The micromechanical properties of the phases have been determined using the nanoindentation data (NanoTest NTX testing centre of Micro Materials Ltd.) after deformation. The results indicate that the interdiffusion of additive atoms have been found during HCV deformation at room temperature. It is shown that the phase's microstructure was homogenized and micromechanical properties changed. We suggesting that are due to result of atoms interdiffusion between different phases, which initiating via microstresses increase during HCV deformation. After deformation appear small pores and defects as result of atoms non balanced interdiffusion. Our experiments have shown the change in atomic order after deformation. We suppose that both the change in atomic order and the shift in the phase equilibria of Ni-based superalloys determine changes in the phase's micromechanical properties and evolution of microstructure characteristics. XRD peaks of the formation of a new proof of the formation of microstructural rafting, defects like micropores and grain boundaries. The material with SC microstructure becomes to polycrystalline microstructure. A mechanism of subsequent fracture includes the above-mentioned phenomena when occur the increasing of cumulative strain during HCV deformation.

Keywords: Order, Ni-based superalloy, interdiffusion, rafting, fracture mechanism