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STUDY OF TEXTURES OF ZIRCONIUM BASED ALLOYS BY NEUTRON AND X-RAY DIFFRACTION

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Introduction

Neutron and X-ray diffraction is a very powerful tool in texture analysis of zirconium base alloys used in nuclear technique [1]. Textures of five samples (labeled as ZZ13, ZZ14, ZZ19, ZZ16 and ZZ17) were investigated by using pole figures and inverse pole figures.

The pole figure measurement were performed at a θ - χ - φ X'Pert PRO diffractometer with CrK α radiation. Pole figures for planes 010 ($2\theta = 48.4^\circ$), 002 ($2\theta = 53.1^\circ$), 011 ($2\theta = 55.6^\circ$) and 110 ($2\theta = 90.4^\circ$) were measured.

The inverse pole figure measurements were performed at diffractometer KSN-2 at Laboratory of Neutron Diffraction, Department of Solid State Engineering, Faculty of Nuclear Sciences and Physical Engineering, CTU in Prague. The wavelength used was $\lambda = 0.1362$ nm. The data were processed using software packages X'Pert Texture, HEXAL [2] and GSAS [3].

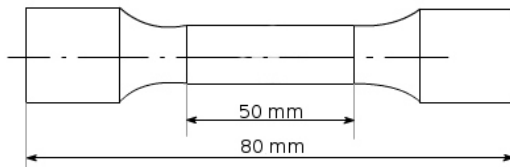


Figure 1. Shape and dimensions of ZZ samples.

Samples

The texture measurements of five samples (labeled as ZZ13, ZZ14, ZZ19, ZZ16 and ZZ17) were performed at the diffractometer KSN-2 at Laboratory of Neutron Diffraction, Department of Solid State Engineering, Faculty of Nuclear Sciences and Physical Engineering using the TG-1 texture goniometer with automatic data collection [2]. The monochromatic neutrons having wavelength 0.1362 nm were used.

Fig. 1 shows shape and dimensions of samples. Four samples (ZZ14, ZZ19, ZZ16 and ZZ17) were deformed by uniaxial tension by using mechanical testing system ISNTRON 5882. Tab. 1 shows parameters of the experiment. Structure of the initial (non-deformed by uniaxial tension) sample ZZ13 observed by using light microscope Zeiss Axio Imager ZM1 and back-reflection X-ray diffraction patterns are in Fig. 2.

Table 1. Parameters of uniaxial tension experiment.

Sample	[%]	[MPa]
ZZ14	6	121
ZZ19	10	124
ZZ16	15	134
ZZ17	20	146

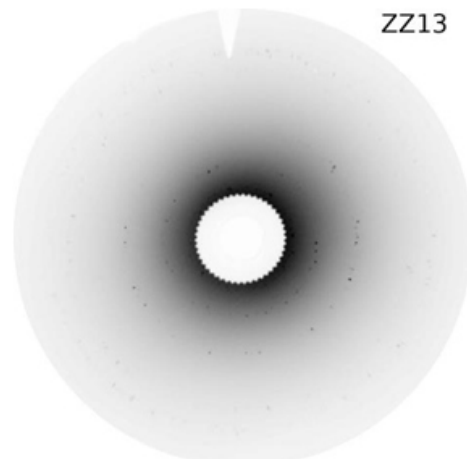


Figure 2. Structure of initial sample ZZ13 observed by light microscope Zeiss Axio Imager ZM1 (left). Back-reflection X-ray diffraction pattern (right).

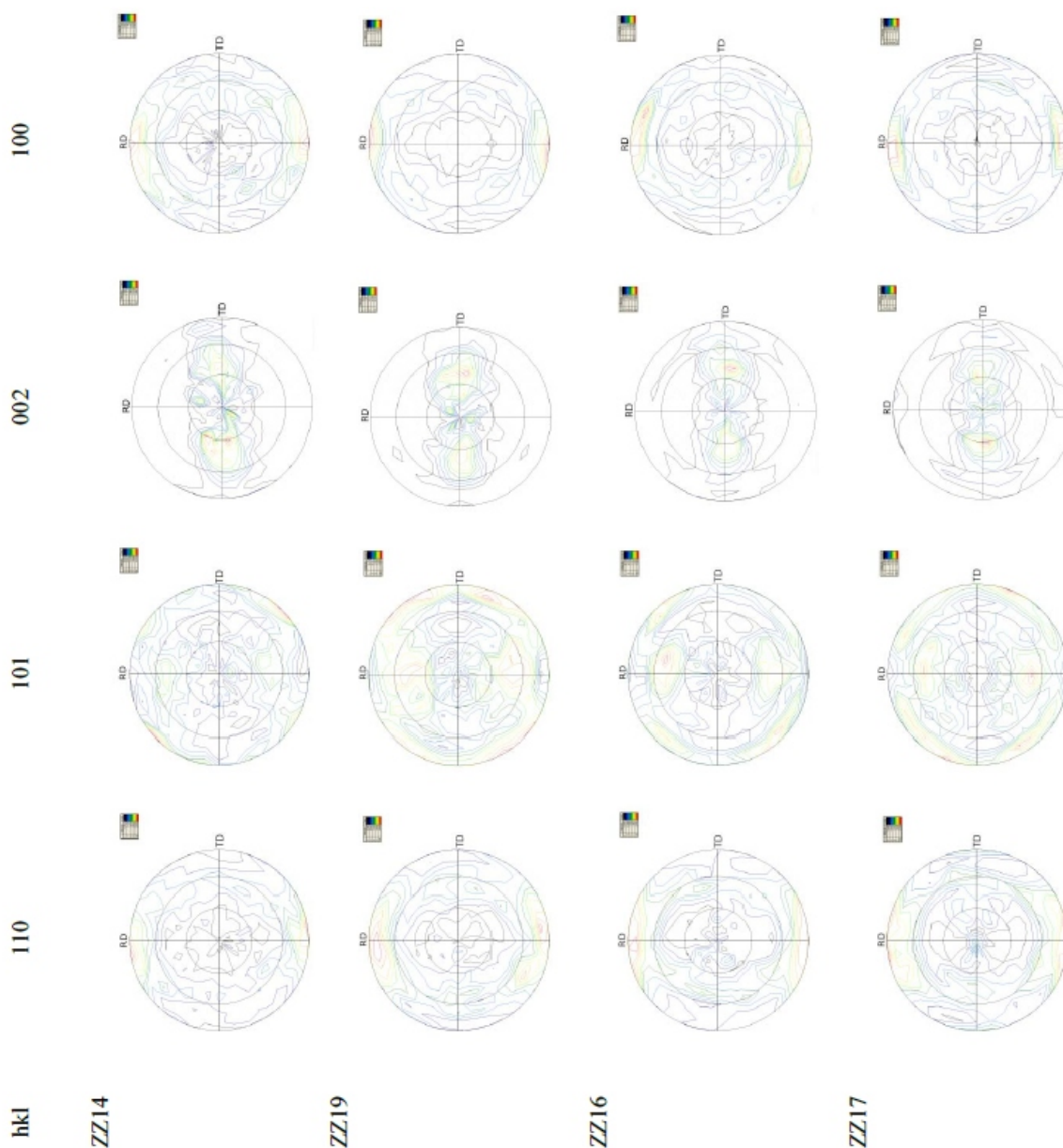
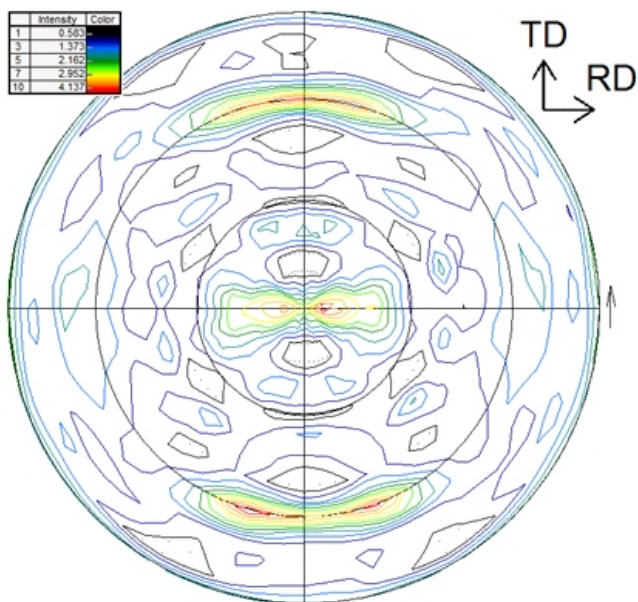


Figure 3. Pole figures of zirconium samples ZZ14, ZZ19, ZZ16 and ZZ17. System of coordinates is represented by ND, RD, and TD.

Table 2. Calculated inverse pole figures of ZZ samples.

Sample	ZZ13	ZZ14	ZZ19	ZZ16	ZZ17
p002, TD	1.3	1.9	1.8	2.1	2.3
p002, ND	2.8	2.7	2.6	2.8	3.1
p002, RD	0.1	0.1	0.1	0	0
p100, TD	1.0	0.7	0.5	0.6	0.5
p100, ND	0.4	0.5	0.4	0.5	0.4
p100, RD	2.6	3.2	4.3	3.8	4.0
p110, TD	0.8	0.8	0.7	0.7	0.9
p110, ND	0.21	0.3	0.2	0.4	0.4



Obr. 1 Přímý pólový obrazec rovin $\{211\}$ měřeného vzorku.

pro výpočet tenzoru zbytkové napjatosti se započítáním přítomnosti textury (určení trojosého stavu napjatosti metodou Winholze-Cohena ale s použitím XSF konstant), viz následující tenzor (2).

$$\begin{pmatrix} 163 & & & & & \\ & 12 & & & & \\ & & 13 & & & \\ & & & 112 & & \\ & & & & 3 & 8 \\ & & & & & 13 \end{pmatrix} \text{ MPa} \quad (2)$$

Z tohoto výsledku je patrné, že v rámci zmíněných aproximací lze stav napjatosti ve vzorku charakterizovat jako dvojosý.

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STUDIUM TEPLOTNÍHO VÝVOJE MŘÍŽKOVÝCH PARAMETRŮ Ni_2MnGa METODOU RENTGENOVÉ DIFRAKCE

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Úvod

Slitiny Ni-Mn-Ga vykazují zajímavé fyzikální jevy, jako je magnetokalorický a elastokalorický jev a tvarová paměť [1]. Bylo objeveno, že některé slitiny typu Ni-Mn-Ga vykazují obří deformaci v magnetickém poli [2]. Tento jev, fundamentálně odlišný od magnetostrické, se nazývá jev magnetické tvarové paměti (Magnetic shape memory – MSM). Uvažuje se, že tento jev by bylo možno využít při konstrukci senzorů či aktuátorů. Proto jsou tyto slitiny v současné době intenzivně studovány.

Pro tyto jevy je nutnou podmínkou martensitický přechod [3]. Tuto změnu lze vyvolat teplotní změnou, tlakem, nebo dokonce magnetickým polem.

Program *stress.m* dle pólové hustoty odhadl podíl texturovaného složky na 81 %. Tato hodnota je dostatečně velká na to, aby tento výsledek mohl být brán v rámci zmíněných aproximací jako korektní. H. Dölle, viz [2], pracuje s hodnotou 80 %. Navíc výpočet proběhl v pořádku, věrohodnost výpočtu byla rovna 0,84 (kde maximum je rovno jedné). Z těchto důvodů lze tento výsledný tenzor brát jako korektní v daném limitním přiblížení textury

Stav zbytkové napjatosti pro předpoklad zanedbání textury, viz (1) se liší od tenzoru s předpokladem přítomnosti textury, viz (2). Důvod je zřejmý; zanedbání vlivu textury. Konkrétně hodnoty normálových napětí σ_{11} , σ_{22} lze v případě předpokladu přítomnosti textury konstatovat významný rozdíl (o 40-50 MPa). Složka σ_{33} je naopak nižší, její hodnota není v rámci chyby statisticky významná. Je patrné, že korekce má v tomto konkrétním případě menší vliv na smykové složky napětí.

Jako vedlejší výsledek byla zjištěna závislost výběru lineárních elastických metod na Millerových indexech a materiálech. Pro roviny $\{211\}$ -Fe je tento výběr bezpředmětný, jelikož se poté dosahuje naprosto stejných výsledků při různých výběrech zmíněných metod. Jiná situace by nastala např. u -Fe pro roviny $\{310\}$, pro roviny $\{211\}$ u jiných materiálů atd.

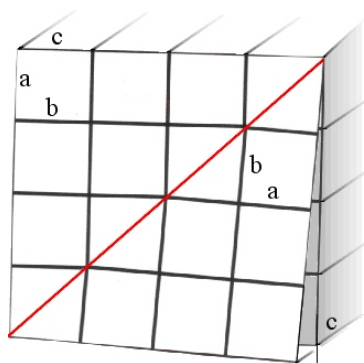
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V dalším textu se budeme zabývat studiem detailního průběhu strukturních změn spojených s tímto přechodem při změně teploty.

Teorie

V Ni_2MnGa dochází při martensitickém přechodu ke změně z kubické mříže na tetragonální, která může vykazovat drobnou ortorombickou či monoklinickou odchylku ($\approx 90^\circ$) [4]. Protože martensitický přechod je fázový přechod 1. druhu, je s ním spojeno latentní teplo a původní i nová fáze mohou ve vzorku koexistovat současně. Díky geometrické neshodě kubické a



Obr 1. Vznik a, b -laminátu dvojčatěním. Diagonála tvoří rovinu dvojčatění. Šedě původní mříž.

tetragonální mříže dochází ke vzniku smykového napětí ve vzorku a ten způsobuje dvojčatění mříže.

Primárně vznikají dvojčata s orientací a a c , sekundárně pak vzniká jemná struktura zvaná a, b -laminát [5]. Rovina dvojčatění zde zrcadlí mřížku tak, že ji otáčí okolo osy c , původní směr strany a přejde na b , zatímco směr strany c zůstává shodný v původní i ozrcadlené mříži. Viz Obr. 1. Jednotlivá dvojčata tvoří ve vzorku tenké vrstvy, odtud tedy název této fáze.

Experiment

Předmětem studia byl monokrystal $\text{Ni}_{50}\text{Mn}_{30}\text{Ga}_{20}$ (at. %) od firmy AdaptMat Ltd. Při daném složení má Ni-Mn-Ga za pokojové teploty pseudotetragonální mříž s mřížkovými parametry $a \sim 0,59$ nm, $b \sim 0,59$ nm, $c \sim 0,56$ nm a $\sim 90^\circ$. Při vyhřátí cca nad 50°C dochází k martensitickému fázovému přechodu a ve vzorku se objevuje austenitická fáze s kubickou mříží s prostorovou

grupou Fm-3m a mřížkovými parametry $a \sim 0,58$ nm a $\sim 90^\circ$.

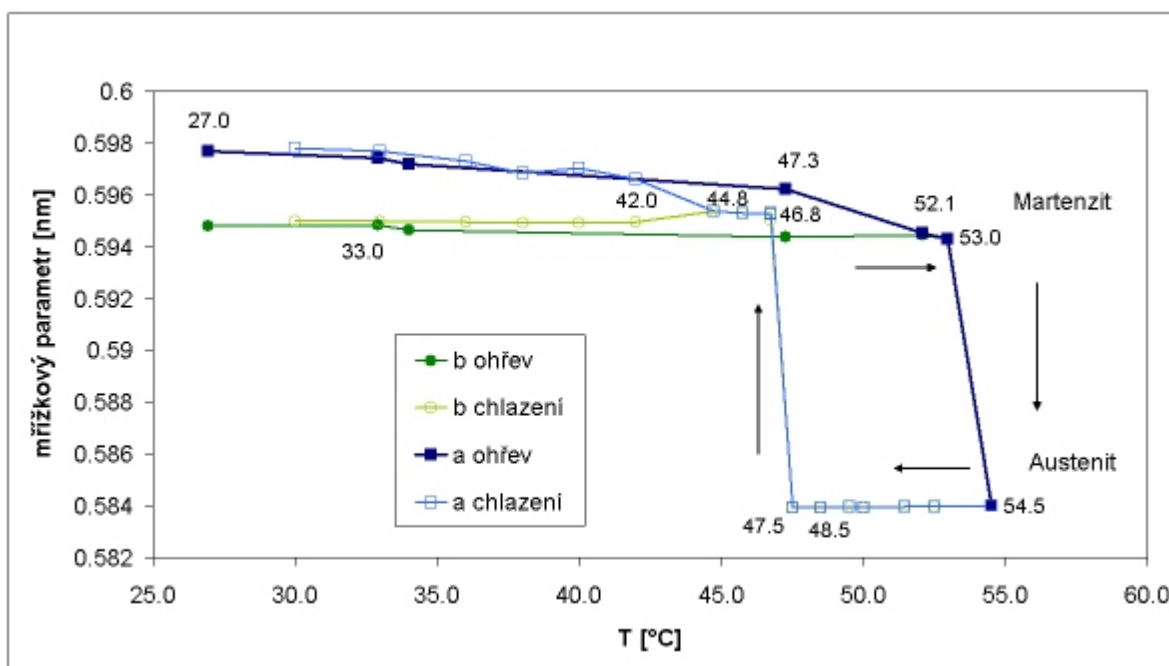
RTG měření proběhlo na horizontálním práškovém difraktometru X'Pert PRO PANalytical. Zdrojem záření byla kobaltová anoda ($\lambda = 1,78901$ Å) s čárovým ohniskem. Při experimentu bylo využito asymetrického Bragg-Brentanova autofokusačního uspořádání pro divergentní svazek. K ohřevu vzorku bylo užito Peltierova článku se zdrojem s měnitelným proudem a napětím.

Výsledky a diskuze

Zkoumali jsme polohu difrakcí 400, 040, 004 v závislosti na teplotě vzorku. Při ohřevu jsme nejdříve pozorovali vzájemně přibližování rozměrů a, b základní buňky, až došlo k jejich ztotožnění na určité hodnotě, která byla blíže rozměru b – mříž tedy přešla na tetragonální symetrii. Při dalším ohřívání dochází ke skokovému přechodu ke kubické austenitické fázi.

Podobné výsledky jsme obdrželi také při měření s klesající teplotou. Austenitická fáze skokově přešla do martensitické fáze s tetragonální symetrií ($a = b$). Při dalším poklesu teploty došlo k rozštěpení na dva různé rozměry a, b . Přechod do martensitické fáze ve směru roviny 004 jsme nepozorovali, vzorek se patrně díky způsobu odvodu tepla a výsledné heterogenní nukleaci vždy zorientoval ve směru rovin 400 a 040 a nikdy nevznikl variant s orientací 004. Teplotní závislost mřížkových parametrů při počáteční orientaci a, b je na obr. 2.

Teplotní křivka při fázovém přechodu vykazuje hysterezi. Velikost hystereze se mírně lišila pro různé počáteční orientace vzorku, což může být způsobeno nedostatečně pomalým ohřevem vzorku, anizotropií teplot-



Obr 2. Vývoj mřížkových parametrů a a b s teplotou. Patrná teplotní hystereze martensitické transformace.



ní vodivosti a závislosti na historii vzorku. Naměřená velikost se pohybuje okolo 6° C.

Závěr

Studovali jsme vývoj pseudotetragonální struktury Ni-Mn-Ga s teplotou. Při martensitickém přechodu do kubické austenitické fáze jsme zaznamenali neznámou mezifázi s tetragonální symetrií. Strukturální přechod je v souladu s teorií martensitické transformace vratný, teplotní křivka při chlazení vykazuje hysterezi o velikosti několika stupňů.

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S9

IMPORTANCE OF XRPD FOR CHEMICAL SYNTHESIS OF OXIDE NANOMATERIALS

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In the recent decade, significant attention has been dedicated to nano-scale materials owing to their interesting physico-chemical or optical properties and possible application as sorbents, catalysts or specialized nanocomposite materials [1]. Chemical approach used to synthesize such materials, very often oxides, may result in the formation of intermediate precursors, whose properties and composition may not be completely understood. In this regard, X-ray powder diffraction (XRPD) serves as very convenient tool for phase identification of prepared materials, determination of crystallite size or other structural properties related to nano-scale materials. A relatively novel approach to synthesize nano-oxides utilizing ionizing or UV radiation has been used by our research group for the preparation of various oxides [2-3]. Recently we also started to investigate mixed oxide systems ($AO_x - BO_y$), where the possibility of solid solution between both terminal oxides significantly complicates the description of the produced nanomaterial. In this regard, XRPD very simply identifies the presence of solid solution and when coupled with any analytical method capable of elemental analysis it can yield exact composition and weight fraction of all phases present in the sample.

The first and also most important purpose of XRPD in analysis of nano-oxide materials is the phase identification with respect to different preparative conditions. Irradiation of e.g. aqueous solution containing zinc nitrate and various other additives by UV light, electron beam or gamma rays can lead to formation of many different products. In the presence of propan-2-ol, hexagonal zinc oxide ZnO, orthorhombic zinc hydroxide $Zn(OH)_2$ (wulfingite) or monoclinic layered hydroxide-nitrate $Zn_5(OH)_8(NO_3)_2$ may be formed (often also a mixture of two phases is produced). Involved mechanism seems to be rather complex and phase identification may thus indicate some possible

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explanations or hints to reactions involved. When hydrogen peroxide ($\cdot OH$ radical source and efficient UV sensitizer) is added to the solution, cubic zinc peroxide ZnO_2 (pyrite structure type) with very small particle size is produced by the irradiation. Addition of formate anion $HCOO^-$ ($\cdot OH$ radical scavenger and photo-active compound) to zinc nitrate promotes the formation of rather small amount of layered hydroxide-carbonate $Zn_5(OH)_6(CO_3)_2$ (hydrozincite), probably due to radiation-induced CO_2 formation from the formate ion. Mild thermal treatment of all produced non-oxide compounds (200 – 400 °C) leads to their decomposition into zinc oxide while retaining their nano-scale character.

Crystallite size of the prepared nanomaterials l can be also determined from powder diffractogram due to the diffraction line broadening. The simplest method involves determination of peak width (FWHM) and using Scherrer equation:

$$l_{hkl} = \frac{K}{\cos \theta_{hkl}}, \quad (1)$$

where K is shape factor (0.89 for spherical particles), λ is radiation wavelength and $\Delta 2\theta_{hkl}$ is the FWHM of selected diffraction line hkl corrected for instrumental broadening. Such a simple size determination is justified by the fact that many oxides produced by radiation method are true nanoparticles with sizes in the range 10 – 50 nm, which was confirmed by other methods such as electron microscopy. Very small spherical nanoparticles with ~ 10 nm diameter are produced in the case of ZnO_2 – consequently, its diffraction lines are very broad and even after its decomposition to ZnO above circa 200 °C the particle size increases only slightly. Most produced compounds such as e.g. syn-

thetic garnets retain their nanoparticle character even after calcination at very high temperatures [3].

Solid solutions of many oxides may be easily obtained when their structure types (or just their lattice systems) are identical – a typical example involves fluorite-type UO_2 and ThO_2 . Due to the different size of U^{4+} and Th^{4+} ions, their lattice constants a differ; when the solid solution is formed, resulting fluorite-type phase has lattice constant a in between UO_2 and ThO_2 . Thus, precise determination of diffraction lines position can be used to estimate the amount of U and Th in the fluorite-type dioxide. Such approach was used for the determination of composition in the radiation-induced preparation of mixed oxide (U,Th) O_2 nuclear fuels, where irradiation of aqueous solution containing uranyl nitrate, thorium nitrate and formate ion causes the formation of an amorphous phase. After calcination at 400 °C or higher in reducing atmosphere, single-phase fluorite-type oxide is formed; diffraction lines positions shift with increasing Th content in aqueous phase indicating efficient incorporation of Th into the mixed oxide.

Solid solutions of oxides with different lattice systems are less common, but can be obtained in specific systems. Irradiation of solutions containing nickel nitrate, zinc nitrate and formate ion induces formation of amorphous solid phase, most probably consisting of mixed (basic) carbonates of Ni and Zn. After mild calcination, halite-type cubic NiO and wurtzite-type hexagonal ZnO are formed, both with very high specific surface area ($> 50 \text{ m}^2 \cdot \text{g}^{-1}$) and small crystallite size. When the Zn content in the aqueous solution is low, only a single phase with cubic lattice is ob-

served by XRPD – the lattice constant a is larger than in the case of pure NiO due to incorporation of larger Zn^{2+} ions into NiO lattice. When the zinc concentration is too high, two separate phases of pure NiO and ZnO are formed. Similar effect may be observed in radiation-induced preparation of ZnO-CdO mixed oxides (CdO has halite structure), where Cd^{2+} may be partially incorporated into hexagonal ZnO (shift of diffraction lines to lower angles 2θ) and simultaneously, Zn^{2+} is present in CdO (shift of CdO diffraction lines to higher angles 2θ). This is more surprising than (Ni,Zn)O solid solution, because CdO has no hexagonal wurtzite-type modification, whereas for ZnO a high-pressure halite-type modification is known.

To conclude, XRPD is an almost irreplaceable and extremely useful analytical method in the field of oxide nanomaterial synthesis, enabling the determination of not only the composition, but also the size of particles and presence of interesting structural effects, most notably solid solutions.

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S10

CREEP TEXTURES OF WATER-WATER NUCLEAR POWER REACTORS CLADDING TUBES MADE OF ZR1NB ALLOY EXAMINED BY NEUTRON DIFFRACTION SUPPLEMENTED BY METALLOGRAPHIC RESEARCH OF HYDRIDES

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Introduction

In nuclear power engineering it is possible to see the tendency to increase the burn-up of nuclear fuel, which leads to more effective fuel utilization and reduces operating costs. However, together with increasing burn-up, the demands on the resistance of the cladding tubes in which the nuclear fuel is encapsulated are increasing. Niobium-alloyed zirconium meets the increasing requirements best.

At elevated temperatures during reactor operation the Zr alloy shows some creep and the cladding tube undergoes changes. The goal of this work was to study creep-caused texture changes in Zr1Nb alloy (also denoted as E-110) by neutron diffraction.

Samples and methods

Tubes composed of Zr and 1 wt % Nb, contain 400 wppm O_2 and 10 – 50 wppm H_2 , too. Tubes were made for fuel rod construction for water-water nuclear power reactors (VVER) and were stored in UJP PRAHA. The outer diameter of tubes prior to deformation was 9,16 mm and their wall thickness was 0,70 mm. Five tubes (samples D, E, F, G, H) of initial length of 100 mm were exposed to 350 – 850 °C and constant tensile stress of 5 – 200 MPa in axial direction (AD). Samples were extended by 36 – 48 %. The atmosphere composed of argon, 10 wppm H_2O , 5 wppm O_2 and 1 wppm CO_2 was used. Traces of water vapour and oxygen caused hydridation and oxidation of the alloy. The experiment was carried out in ÚFM AVČR [1]. The texture was analyzed by KSN-2 diffractometer, thermal neutrons were produced by LVR-15 reactor in Nuclear Research In-



stitute in Řež u Prahy. The results were plotted as inverse pole figures calculated by Harris method [2, 3]. The hydrides were documented on metallographic polished sections in UJP PRAHA.

Changes of texture and reorientation of hydrides

Temperatures corresponding to VVER operation temperature or higher, combined with constant tensile stress, cause creep leading to increased formation of zirconium crystallites, which rotate their bases in a direction perpendicular to tangential direction (TD). This represents conditions favourable for hydride precipitation in the radial direction (RD), which dramatically reduce tube wall resistance to rupture. However, this effect was observed during experiments with open tubes without internal overpressure. Under real operation conditions in a reactor, the overpressure of gasses inside the fuel rod contributes to the deformation of cladding tubes. Results of Rogozyanov et al. [4] suggest that in standard operation conditions of VVER, the effect of axial tensile stress slightly dominate over the internal overpressure effects. The final deformation is approx. 80 x smaller than the deformation resulting from performed experiments and resulting texture changes will have only small influence on the orientation of hydrides. Distinctive unfavourable changes in hydride orientation can be expected only during accident of cask/container accompanied by temperature rise and break of the cask/container.

The orientation of hydrides did not changed continuously: hydride orientation is usually random and directional alignment was found only in extremely deformed tubes, where the pole density (p') of plane (100) in AD exceeded the boundary which lies in the interval 6,9 – 8,6.

New texture

In cladding tubes exposed to 700 °C and constant tensile stress of 10 MPa for 184 h (sample G), a new (not yet described in literature) texture appeared: the highest pole density (p') in TD was found for (101) pyramid followed by p' for (100) prism. This texture can be explained by {111} twinning, as only this twin can face both (101) and (100) planes perpendicular to TD. Moreover, only in this sample the (110) prism shows the highest p' in AD of all of the observed planes in this sample, while the (100) prism has the lowest p' compared to all samples. High p' of the (110) prism and the occurrence of {111} twinning prove recrystallisation. Reversible phase transformation of a significant amount of α -Zr - β -Zr probably contributes to the formation of this new texture.

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S11

STRUCTURE AND FUNCTION OF BACTERIAL NUCLEASES

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Keywords: nucleases, protein crystallography, single-wavelength anomalous dispersion

Abstract

Nucleases are a broad group of enzymes which controls hydrolysis of phosphodiester bonds in nucleic acids. The reaction is used in wide spectrum of biological processes, which is in correlation with number of different structures and reaction mechanisms. Nucleases play their role in DNA replication, transcription from DNA to RNA, nucleic acid's repairs, apoptotic processes and controlled cell death or in degradation of nucleic acids as a nutrition source. The reaction mechanisms are possible to characterise with respect to reaction centre constitution, presence of metal ions, deprotonated water or typical amino-acid residues as

serine, thyrrosine or histidine. One of the bacterial nucleases was successfully crystallized and diffraction data were collected. A phase problem solution is in progress.

Introduction

Nucleases are a group of enzymes responsible for cleavage of DNA and RNA. The reaction is involved in various biological processes: DNA replication, recombination, reparation processes, nucleic acids (NA) degradation, programmed cell death, etc. Different requirements on nucleases function leads to structural and reaction mechanisms diversity. As nucleic acids are an essential compound of living beings, their degradation is fatal. Therefore, production and function of nucleases is strongly regulated in cells.