



# Straightforward understanding of the structures of metastable $\alpha''$ and possible ordered phases in uranium–niobium alloys from crystallographic simulation



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## ABSTRACT

Crystallographic simulation is carried out in the present work to understand the respective structure of metastable  $\alpha''$  and possible ordered phases, which could be the prerequisite for revealing the low-temperature aging mechanism underlying the  $\alpha''$  phase in U–Nb alloys. The space group of No. 11 with C-type lattice is found to describe the structure of  $\alpha''$  phase in a straightforward way, avoiding the mistaken or indirect indexation and analysis of structural data. The obtained theoretical diffraction pattern of  $\alpha''$  phase shows clearly the phenomenon of peak splitting, in which the Bragg positions also agree well with the experimental observation. Additional peaks are observed at the low diffraction angles for the possible ordered phases in U–Nb alloys through simulation on the proposed two types of structures, which need to be carefully detected by the uniting of multiprobe diffraction. The correlation between ordered structures and stress-strain response is also deduced and discussed. The present work would provide some enlighten to the integrity of the phase diagram and the understanding of low-temperature aging mechanism in U–Nb alloys.

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## 1. Introduction

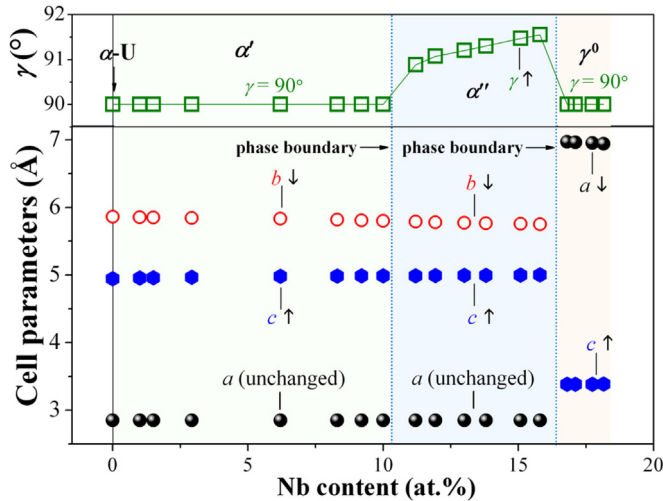
Uranium metal and alloys have been of both scientific interest and technologic importance for a long time [1–4], which have found many applications in the nuclear weapon and energy systems. Uranium–niobium (U–Nb) are good candidate for structural materials in weapon system due to their excellent mechanical and corrosion-resistant properties [5,6]. The addition of niobium into uranium metal enriches the categories of phases, which include the equilibrium (i.e.,  $\alpha$ ,  $\beta$ , and  $\gamma$ ) and metastable (usually symbolized as  $\alpha'$ ,  $\alpha''$  and  $\gamma^0$ ) ones. The metastable phases (i.e., extended solid solutions) are produced during the cooling of stable  $\gamma$  phase from relatively high to room temperature at a rapid rate (e.g., water quenched). The evolution of metastable phases behaves as a function of Nb content [7], as shown in Fig. 1. Both  $\alpha''$  and  $\gamma^0$  phases show the obvious shape memory effect (SME) like the Ni–Ti alloys. Near the phase boundary between  $\alpha''$  and  $\gamma^0$ , the U–Nb alloys are considered

the most excellent candidate for structural components due to the enhanced SME. Those alloys show a dual-yielding deformation behavior, and much attention is paid on the underlying mechanism in the microscale. For instance, the lattice strain response of the  $\alpha''$  and  $\gamma^0$  phases for bulk U–Nb alloys under different deformation states has been investigated online through neutron diffraction [8–10], and the evolution of fraction volume for these two phase has been also acquired during the stress-induced phase transition from  $\alpha''$  to  $\gamma^0$ . However, due to the metastability of those phases, low-temperature aging can significantly influence their mechanical properties. Briefly, the SME is weakened after low-temperature aging with the decrease of ductility. There is still a controversy on the mechanism of low-temperature aging, while that of high-temperature aging is already illuminated and clarified. When aged at a relatively high temperature ranging from about 300 °C to 500 °C,  $\alpha''$  phase transforms partially to be  $\gamma^0$  phase. The reversible transition (i.e., from  $\gamma^0$  to  $\alpha''$ ) can be induced by stress. When the aging temperature is higher than 500 °C,  $\alpha''$  phase decomposes into cellular  $\alpha$  and  $\gamma$  dual-phases. And for the low-temperature (<300 °C) aging, some investigations have attempted to explain this mechanism from different aspects of spinodal decomposition, chemical redistribution and phase transformation [11–13], however, without sufficient or convincing evidences. Presently, it is still

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**Fig. 1.** Cell parameters for metastable  $\alpha'$ ,  $\alpha''$  and  $\gamma^0$  phases as a function of the content of Nb. The vertical dotted lines indicate the phase boundary between  $\alpha'$  and  $\alpha''$ , and between  $\alpha''$  and  $\gamma^0$ . The arrow beside the cell parameters  $a$ ,  $b$ ,  $c$  and angle  $\gamma$  indicates the increase (up) or decrease (down) of them with increasing the content of Nb. The data of cell parameters are generally taken from Ref. [7].

unclear how the structure of  $\alpha''$  phase exactly changes during the low-temperature aging. Thus, for the understanding of the low-temperature mechanism, clarifying two points could be useful, which are respectively the structures of  $\alpha''$  and the possible ordered phases. However, the structural information such as the space group for  $\alpha''$  phase is not clearly stated in a straightforward way, although it is thought to be monoclinic (i.e., distorted from  $\alpha$  phase) and its cell parameters (i.e., the lattice constants  $a$ ,  $b$ ,  $c$ , and the angle  $\gamma$ , as shown in Fig. 1) have been provided. For this reason, the analysis on structure of  $\alpha''$  phase is usually performed in an indirect or incorrect way. For example, in a current and early work [13,14], diffraction pattern of  $\alpha''$  phase is indexed by the orthorhombic and triclinic  $\alpha$  lattice, respectively.

The ordering effect is naturally connected to the aging mechanism, which is suggested by Hsiung for U–Nb system [11], however, only the illustrative schemes of the ordered structures are provided but without further evidences. Anyway, it is a kind reminder for us to review the phase diagram of U–Nb binary system [15], which is still blank in the region of relatively low temperatures. Paying attention to other similar U–X (X represents the neighboring elements such as Ti, Zr and Mo) systems, it can be noticed that all of them have ordered intermetallic phases, as seen in Fig. 2. The 2:1, 1:2 and 2:1 type of ordered phase is respectively found in the U–Ti, U–Zr and U–Mo system [16]. It implies that the ordered phase might also exist in the U–Nb system from the viewpoint of neighboring effect, which will contribute to the integrity of the corresponding phase diagram, simultaneously, to the understanding of low-temperature aging mechanism.

Therefore, the present work focuses on the respective structure of metastable  $\alpha''$  and the possible ordered phases through crystallographic simulation. With the proper space group, the structure and theoretical diffraction pattern of  $\alpha''$  phase are clearly achieved in a straightforward way. The possible ordered phase is discussed based on the structure construction and multiprobe (i.e., x-ray, neutron and electron) diffraction simulation, which would shine some light on the understanding of the ordered phases and thus the mechanism of low-temperature aging in U–Nb alloys.

## 2. Computational details

The principle of x-ray and neutron diffraction is similar with each other. The feature of the diffraction patterns may be typically described by positions, intensities and shapes of multiple Bragg reflections disregarding the background. The diffraction patterns are usually a function of the crystal structure, specimen and instrumental parameters. The intensity,  $I(hkl)$ , scattered by a reciprocal lattice point ( $hkl$ ) corresponding to the integrated intensity of the Bragg peak, is a function of the atomic structure and it also depends on multiple factors. Its computational expression includes the scale, multiplicity, Lorentz, polarization, absorption, preferred orientation, extinction and structure factors [17]. In the present work, under the assumption of ideal crystals, and neglecting the sample-relative factors like preferred orientation and absorption factors, the intensity,  $I(hkl)$ , can be then simplified as

$$I(hkl) = |F_{hkl}|^2 Lp(\theta), \quad (1)$$

where  $\theta$  is the Bragg angle,  $F_{hkl}$  denotes the structure factor, and  $Lp(\theta)$  represents the Lorentz-polarization factor that depends on the diffraction geometry and radiation. Expressions for those factors mentioned above have been given elsewhere [17,18]. For calculation, the intensity in the diffraction patterns can be written as

$$I^{cal}(2\theta) = \sum_{2\theta} I_n(hkl) f_n(2\theta) + B(2\theta), \quad (2)$$

where  $2\theta$  is the diffraction angle,  $I_n(hkl)$  denotes the intensity for the  $n$ th Bragg peak, and  $f_n(2\theta)$  and  $B(2\theta)$  represents the peak shape and background function, respectively. In brief, when calculating the neutron and x-ray diffraction patterns, the structure (e.g., space group, lattice constant, atoms' type, coordinate and occupation) and instrument (e.g., wavelength of the radiation) parameters are input, as well as the peak shape function, and then the diffraction patterns are achieved and output through the programs such as FullProf Suite [19], CrystalDiffract<sup>®</sup> and VESTA (Visualization for Electronic and Structural Analysis) utilizing RIETAN-FP [20]. The program uses automatically the atomic scattering factors (for x-ray diffraction) or neutron scattering lengths of the atoms (for neutron diffraction) in the defined structure. The structure parameters used in the calculation are taken from the data as given in Fig. 1. The background level  $B(2\theta)$  is set to be zero, and both the wavelength of x-ray and neutron is assumed to be 1.6 Å. The Gaussian function is used as the peak shape function. The three-dimensional (3D) and two-dimensional (2D) visualizations for the crystal structure are displayed by the VESTA. For solid solutions, the addition of alloying elements doesn't change the main crystal structure of uranium. From this viewpoint, only the uranium atom is displayed in the crystal structures in the following text.

From the viewpoints of kinematics, the principle of electron diffraction is very similar with that of x-ray diffraction, which also obeys the Bragg's law and Laue equation. Therefore, the reciprocal lattice can be used to represent the electron diffraction pattern to some extent. In the present work, the weighted reciprocal lattice (WRL) is shown by the program of Reciprocal Lattice Visualizer in the FullProf Suite. The electron diffraction patterns can also be directly visualized through the program of SingleCrystal<sup>™</sup>, which are consistent with those through Reciprocal Lattice Visualizer.

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