

Deformation-induced ω phase in nanocrystalline Mo

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A deformation-induced hexagonal ω phase was first observed in pure nanocrystalline body-centered cubic (bcc) Mo using high-resolution transmission electron microscopy. As the grains were refined into nanometer sizes by deformation using high-pressure torsion under a pressure of ~ 4 GPa at room temperature, the ω phase formed at the grain boundaries of bcc Mo with a crystallographic relationship close to the $\{112\}\langle 111\rangle$ twin orientation. Its formation was mainly attributed to the shear deformation on $\{112\}$ planes in bcc Mo.

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The hexagonal ω phase (space group: $P6/mmm$) is a widely studied metastable phase in numerous group IV and V transition metals (Ti, Zr, Hf and Ta) and their alloys [1–12]. It is formed from a hexagonal α phase or a body-centered cubic (bcc) β phase through phase transformation during high-temperature aging or under static/dynamic pressure. This phase transformation is of great interest because it could provide an additional strengthening mechanism for these materials [4,6]. Previous studies have revealed that the ω phase transformation is very common in β -Ti alloys during heat treatment or conventional mechanical deformation [9–11]. Its existence would greatly improve the alloy's mechanical properties, such as ultralow elastic modulus and ultrahigh strength. In addition, shock-induced ω phase transformation has been reported in polycrystalline Ta and its alloys that were shock-deformed at a very high pressure (~ 45 GPa) [12]. It is suggested that the shear deformation on $\{112\}$ planes is the main mechanism for the formation of ω phase.

Refining the grains of materials into nanometer sizes can significantly alter the physical, chemical and mechanical behavior of the materials [13–22]. For example, nanocrystalline (nc) Cu and Ni have displayed superior strength with good ductility when their deformation is significantly controlled by twins and partial dislocation emission at the grain boundaries [13–15]. Nanoscale

grain size also has a significant effect on the phase transformation in metals and alloys [23–25]. Wang et al. [25] have investigated the grain size effects on reversible β -to- ω phase transformation in a Ti-based alloy processed by high-pressure torsion (HPT). The ω phase occurred at the initial stage but disappeared when the grain size decreased to ~ 50 nm.

In this paper, we report a deformation-induced ω phase transformation in pure nc Mo processed by HPT under a pressure of ~ 4 GPa at room temperature. Mo has a bcc structure (space group: $Im\bar{3}m$; $a = 0.3147$ nm [26]), and exhibits no equilibrium phase transformation up to its melting temperature at ambient pressure. To date, no reports have been published on the ω phase in pure Mo. Here we investigate for the first time the morphology, formation mechanism and interfacial structure of the ω phase in nc Mo.

Sample disks, 0.76 mm thick and 10 mm in diameter, were cut from an Mo sheet and deformed using HPT for six turns under a pressure of 4 GPa. A detailed description of HPT procedure can be found elsewhere [27,28]. Wedge-shaped thin foils for transmission electron microscopy (TEM) observations were sampled from the edge of HPT-processed Mo disks. TEM and high-resolution TEM (HRTEM) observations were carried out using a JEOL 2010F microscope operating at 200 kV. HRTEM image simulations were performed using the EMS software package.

TEM investigations revealed an average grain size of ~ 90 nm in nc Mo, based on at least 500 randomly selected

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grains. A typical deformation microstructure of nc Mo is shown in Figure 1a. From the corresponding selected area diffraction (SAD) pattern in Figure 1b, the two marked lattices (A and B, both in $[1\bar{1}0]$ zone axes from bcc Mo) are from the grains marked A and B in Figure 1a, respectively. They can be clearly distinguished in the two dark-field TEM images in Figure 1d and e, respectively. From the composite SAD pattern in Figure 1b, the angle between the two (110) planes of lattices A and B are $\sim 67.3^\circ$, which is very close to the 70.5° angle of a twin relationship in bcc systems.

In addition to grains A and B, there is also an intergranular phase with a width of ~ 30 nm between them, which is framed by the white solid line (zone C) in an enlarged image in Figure 1f based on HRTEM observations. It is identified to be a ω phase according to the fast Fourier transform (FFT) diffraction pattern in Figure 1c, which is directly taken from an HRTEM image corresponding to the framed rectangular zone I in Figure 1f. Here the $[2\bar{1}\bar{1}0]_\omega$ zone diffraction patterns of the ω phase are superimposed with the $[1\bar{1}0]_\alpha$ zone diffraction pattern of the parent α phase (we call the bcc Mo phase the α phase). The orientation relationship between the ω and α phases is determined to be: $[2\bar{1}\bar{1}0]_\omega // [1\bar{1}0]_\alpha$ and $(01\bar{1}0)_\omega // (11\bar{2})_\alpha$. The lattice parameters of the ω phase are $a_\omega = \sqrt{2}a_\alpha = 0.445$ nm and $c_\omega = \sqrt{3}a_\alpha/2 = 0.273$ nm ($c/a = 0.613$). The ω phase is distributed continuously at the intergranular zone (zone C), with an irregular shape between grains A and B, as shown in Figure 1d–f. This is completely different from the observations in previous studies [4,12,25], which reported that the ω phase always occurs in the bcc phase in a plate-like or cuboidal shape.

The existence of ω phase in nc Mo is further verified by HRTEM micrographs in Figure 2. Figure 2a displays an experimentally observed HRTEM image of ω phase taken from the $[2\bar{1}\bar{1}0]_\omega$ zone axis, in which the dots show

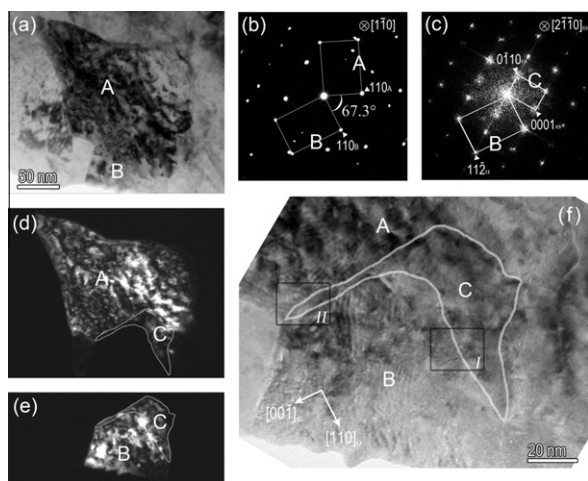


Figure 1. Bright-field (a and f) and dark-field (d and e) TEM images showing the typical morphology of ω phase in nc Mo. The related grains are marked by A, B and C, respectively. (b) A composite SAD pattern corresponding to (a); (c) an FFT diffraction pattern of α and ω phases taken from an HRTEM image corresponding to the framed zone I in (f). Both (110) spots of lattices A and B in (b) were used to take the two dark-field images (d and e, respectively).

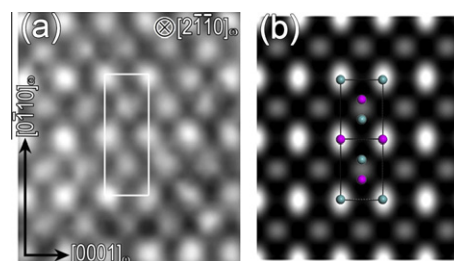


Figure 2. HRTEM investigations of ω phase in nc Mo, taken from the $[2\bar{1}\bar{1}0]_\omega$ zone axis. (a and b) Experimental and simulated (defocus = 4 nm, thickness = 8 nm) images of ω phase, respectively. The atomic projection of an ω unit cell is given in (b).

periodic bright and weak configurations along the $[0\bar{1}10]_\omega$ direction. Figure 2b shows a simulated HRTEM image of ω phase in the same zone axis obtained at a defocus of ~ 4 nm and a thickness of ~ 8 nm. From the atomic projection of an ω unit cell in Figure 2b, the two atomic columns in the ω structure can only display one weak spot in the simulated image under the current image conditions. Thus, the simulated result agrees well with the experimental image.

In order to investigate the formation mechanism of the ω phase, Figure 3a presents a schematic illustration of the crystallographic relationship between the ω and α phases. The marked hexagonal ω lattice can be completely contained in the $2 \times 3 \times 2$ α superlattice. The occupancies of the atoms in the ω lattice points are on the sites of the atoms in the α superlattice. However, the sites of the two marked atoms A and B must be moved a distance of $1/12[111]$ along the $[111]$ and $[\bar{1}\bar{1}\bar{1}]$ directions ($A \rightarrow A'$ and $B \rightarrow B'$), respectively, to form a hexagonal ω structure. The transformation process is clearly illustrated in Figure 3b, which displays a two-dimensional atomic projection of the ω (upper) and α (bottom) phases taken from zone axes of $[2\bar{1}\bar{1}0]_\omega // [1\bar{1}0]_\alpha$. Both ω and α phases have six atomic layers (marked in Fig. 3b) along the $[0\bar{1}10]_\omega$ and $[\bar{1}\bar{1}\bar{2}]_\alpha$ directions, and two layers along the projected directions. The marked atoms A and B at the bottom of Figure 3b correspond to the two atoms A and B in Figure 3a. The ω phase can be formed when the atoms (A and B) in layers 2 and 3 of the α phase shuffle $1/12[111]$ along the

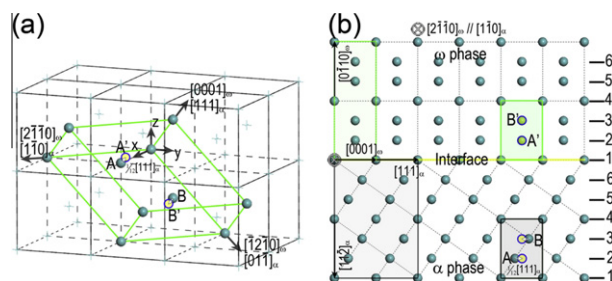


Figure 3. Illustration of the formation mechanism of ω phase in nc Mo. (a) Schematic showing the crystallographic relationship between the ω and α phases. (b) Composite atomic model illustrating how to form hexagonal ω phase (upper) from bcc α phase (bottom), viewed from the zone axes of $[2\bar{1}\bar{1}0]_\omega // [1\bar{1}0]_\alpha$.

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