Prediction and Mechanism of Tensile Strengthening in Single β-phase Ti-Ta Alloys with Oxygen Solutes

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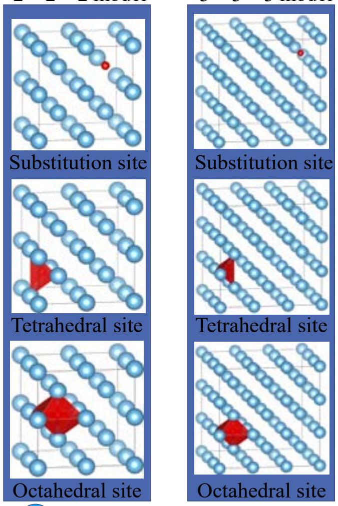
Introduction

Oxygen solid solution is known as one of strengthening mechanisms in Ti alloys. The lattice distortion owing to solid solution is the key point in this strengthening mechanism and can be theoretically analyzed by first-principles calculations. In this poster, the local structure of solutes oxygen and the lattice distortion in β-Ti alloy model were computationally elucidated by using first-principles calculations. In addition, the increment of 0.2% yield strength of β-Ti alloy model was estimated by combining these results with the Labusch model, the theory of solid solution strengthening. These increments of 0.2% yield strength were validated by experiments. The single β-phase Ti alloys with various oxygen concentrations were fabricated by powder metallurgy and a series of heat treatment, and their microstructure and mechanical properties were characterized.

Calculation conditions



First-principles calculations

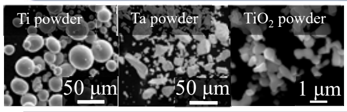
- VASP code
- Cutoff energy : 520 eV
- K-point spacing : 0.15 Å^{-1}

Labusch model

$$\Delta\sigma_{YS} = \frac{\tau_0}{S_F} = \frac{1}{S_F}\left(\frac{F_m{}^4 c^2 w}{4Gb^9}\right)^{\frac{1}{3}}$$

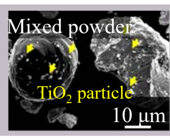
τ_0 : Shear stress
S_F : Schmid factor
F_m : Maximum interaction force between solute atom and dislocation
c : Solute atom concentration
w : The range of the interaction
G : Modulus of rigidity
b : Burgers vector size

Experimental procedure

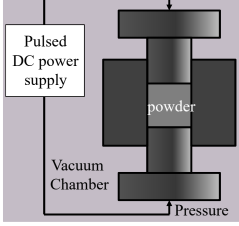


Ti-35Ta+xO
x=1.5, 2.4, 3.6 at.%

① Mixing
Ball milling : 1 hr
Rocking milling : 3 hr



② Spark plasma sintering (SPS)



Temp. : 1373 K
Time : 1 hr
Pressure : 30 MPa
Diameter : 42 mm

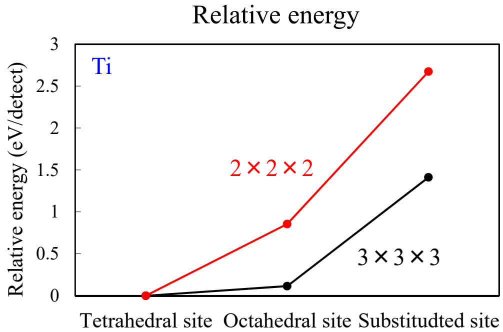
③ Homogenizing
Temp. : 1773 K
Time : 12 hr

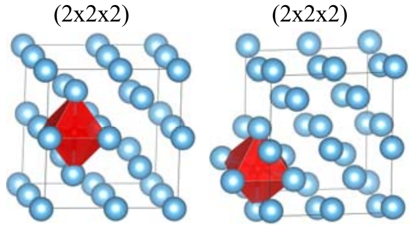
④ Hot forging
Temp. : 1373 K
Time : 5 min
Load : 1650 kN

⑤ Quenching
Temp. : 1773 K
Time : 1 hr

Results –lattice distortion and mechanical properties

Theoretical results by using First-principles calculations and the Labusch model



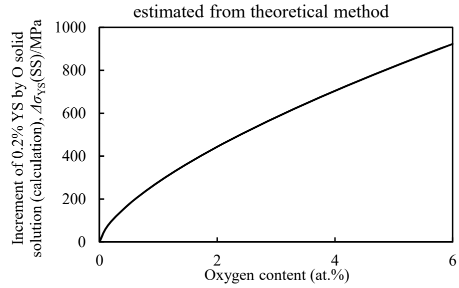


Solute oxygen is most stable at the octahedral site in both results.

Labusch model

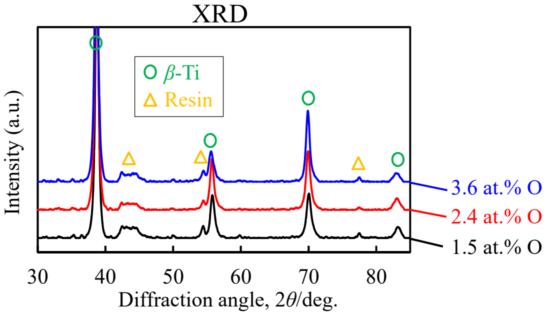
$$\Delta\sigma_{YS} = \frac{\tau_0}{S_F} = \frac{1}{S_F}\left(\frac{F_m{}^4 c^2 w}{4Gb^9}\right)^{\frac{1}{3}}$$

Increment of 0.2%YS by solid solution estimated from theoretical method

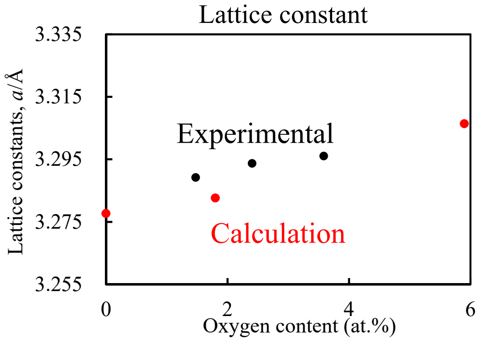


Increment of 0.2%YS by O solution could be theoretically estimated.

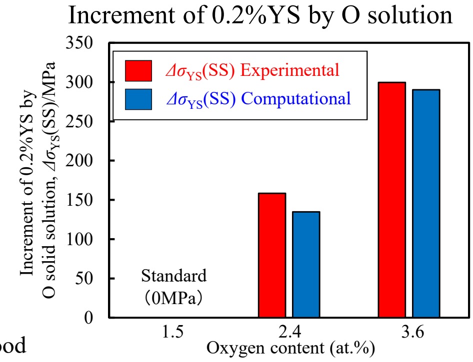
Validation by Experiments



Fabricated specimens have single β phase.



The experimental lattice constants are in a good agreement with calculation results.



The increments of 0.2% YS were validated.