Microstructural Evolution and Reaction Mechanisms of the Ti/ZrO_2 Interface between 1100° and 1550°C

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Abstract

The diffusional reaction between titanium and zirconia was carried out isothermally in argon at temperatures range from 1100° to 1550°C. The distinct reaction layers between titanium and zirconia were investigated using electron probe microanalyses (EPMA), analytical scanning electron microscopy (SEM), and analytical transmission electron microscopy (TEM) both attached with an energy-dispersive spectrometer (EDS). After annealing at 1100°C/6 h, a lamellar of Ti_2ZrO and α-Ti(O, Zr) phases were found in the interface, while zirconia grains did not grow conspicuously. At 1300°C, a lamellar of Ti_2ZrO + α-Ti(O, Zr) and β'-Ti (Zr, O) were found in the titanium side. The α-Zr excluded from *t*-ZrO_{2-x} in the zirconia side during cooling. At 1400°C, lamellar of Ti_2ZrO + α-Ti(O, Zr), acicular α-Ti (O, Zr) + β'-Ti (O, Zr), and continuous β'-Ti (Zr, O) layers were found in the titanium side. The acicular α-Ti(Zr, O) was precipitated from β'-Ti(Zr, O) matrix by means of the ledge mechanism. The acicular α-Ti and the β'-Ti showed two different orientation relations: one was $[2\bar{1}\bar{1}0]_{\alpha\text{-Ti}}$ // $[001]_{\beta'\text{-Ti}}$ and $(0001)_{\alpha\text{-Ti}}$ // $(100)_{\beta'\text{-Ti}}$, and the other was $[2\bar{1}\bar{1}0]_{\alpha\text{-Ti}}$ // $[021]_{\beta'\text{-Ti}}$ and

$(0001)_{\alpha\text{-Ti}}$ // $(1\bar{1}2)_{\beta'\text{-Ti}}$. After annealing at 1550°C, four layers in a sequence of Ti_2ZrO + α-Ti(O, Zr), Ti_2ZrO + α-Ti(O, Zr) + β'-Ti (O, Zr), acicular α-Ti (O, Zr) + β'-Ti (O, Zr), and continuous β'-Ti (Zr, O) were formed in the titanium side after cooling. The lamellar and the spherical Ti_2ZrO, which were orthorhombic and hexagonal, respectively, were found. The spherical hexagonal Ti_2ZrO was an ordered structure, with zirconium and oxygen occupying substitutional and interstitial sites, respectively. The orientation relations between α-Ti and the lamellae orthorhombic Ti_2ZrO were determined to be $[0001]_{\alpha\text{-Ti}}$ // $[110]_{Ti2ZrO}$ and $(10\bar{1}0)_{\alpha\text{-Ti}}$ // $(1\bar{1}0)_{Ti2ZrO}$; meanwhile those between the α-Ti and the spherical hexagonal Ti_2ZrO were $[0001]_{\alpha\text{-Ti}}$ // $[0001]_{Ti2ZrO}$ and $(10\bar{1}0)_{\alpha\text{-Ti}}$ // $(10\bar{1}0)_{Ti2ZrO}$. In the zirconia side, when held above 1400°C, two reaction layers were found: near the original interface, β'-Ti coexisted with fine spherical *c*-ZrO_{2-x} and Chinese-script-like *c*-ZrO_{2-x}, which dissolved a significant amount of Y_2O_3 in solid solution; further away from the original interface, the coarsened intergranular α-Zr was excluded from metastable ZrO_{2-x}, resulting in the lenticular *t*-ZrO_{2-x} and ordered *c*-ZrO_{2-x}. The ordered *c*-ZrO_{2-x} was identified by the 1/5{113} superlattice reflections of its electron diffraction patterns. The microstructural developments and reaction mechanisms in the Ti/ZrO_2 diffusion couples annealed for various temperatures were described by the aid of the Ti-Zr-O ternary phase diagram.