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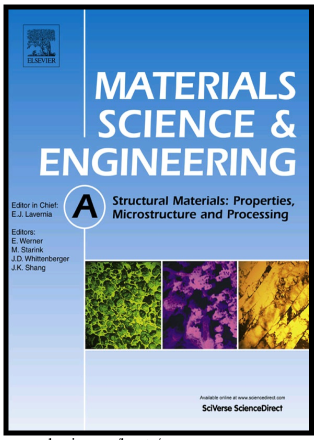

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Coupled strain-induced alpha to omega phase transformation and plastic flow in zirconium under high pressure torsion in a rotational diamond anvil cell

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Abstract

Strain-induced $\alpha \rightarrow \omega$ phase transformation (PT) in the zirconium (Zr) sample under compression and plastic shear in a rotational diamond anvil cell (RDAC) is investigated using the finite element method (FEM). The fields of the volume fraction of the ω phase, all components of the stress tensor, and plastic strain are presented. Before torsion, PT barely occurs. During torsion under a fixed applied force, PT initiates at the center of the sample, where the pressure first reaches the minimum pressure for strain-induced $\alpha \rightarrow \omega$ PT, p_ε^d, and propagates from the center to the periphery and from the symmetry plane to the contact surface. Salient increase of the shear friction stress and pressure at the center of a sample, so-called pressure self-multiplication effect observed experimentally for some other materials, is predicted here for Zr. It is caused by much higher yield strength of the ω phase in comparison with the α phase. Except at the very center of a sample, the total contact friction stress is equal to the yield strength in shear of the mixture of phases and the plastic sliding occurs there. Due to the reduction in sample thickness and radial material flow during torsion, the ω phase can be observed in the region where pressure is lower than p_ε^d, which may lead to misinterpretation of the experimental data for p_ε^d. For the same applied force, torsion drastically promotes PT in comparison with the compression without torsion. However, the PT process in RDAC is far from optimal: (a) due to the pressure self-multiplication effect, the pressure in the transformed region is much higher than that required for PT; (b) the region in which PT occurs is limited by the pressure p_ε^d and cannot be expanded by increasing a shear under a fixed force; and (c) the significant reduction in thickness during torsion reduces the total mass of the high-pressure phase. These drawbacks can be overcome by placing a sample within a strong gasket with an optimized geometry. It is shown that, due to strong pressure heterogeneity, characterization of $\alpha \rightarrow \omega$ and $\alpha \rightarrow \beta$ PTs based on

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