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Room-Temperature Plasticity in ZrC: Role of Crystal Anisotropy

CHRISTIAN RATSCH, S. KIANI, A.M. MINOR, S. KODAMBAKA, J.M. YANG, UCLA — NaCl structure Group IV and V transition-metal carbides are hard, stiff, and high-melting solids with excellent wear, abrasion, and corrosion resistances, and are commonly used in advanced high-temperature structural applications. In this talk, we report results obtained from in situ transmission electron microscopy (TEM) studies and density functional theory calculations of uniaxial compression of ZrC(100) and ZrC(111) single crystals. In situ TEM observations show that dislocation motion and tangling lead to plastic deformation in ZrC(111), while slip along {110}<1-10>is dominant in ZrC(100). We find that the yield strengths of ZrC crystals increase with decreasing size. Interestingly, yield strengths of uniaxially compressed ZrC(111) crystals are lower than those of ZrC(100), unexpected for NaCl-structured compounds. Based upon density-functional theory calculations, we attribute the orientation-dependent yield strengths to relatively lower energy barrier for shear along {001}<1-10>compared to {110}<1-10>. Our results provide important insights into the effects of crystal size and orientation on room-temperature plasticity. We expect that similar phenomena are likely to exist in other cubic-structured transition-metal carbides and nitrides.

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