

Valence Electron Concentration can be Adjusted to Increase Plasticity in High-Entropy Refractory Ceramics

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Abstract

A possible method for creating materials with a rare combination of high hardness and fracture-resistance at high temperatures is bottom-up design of high-entropy ceramics. This work provides a straightforward yet fundamental design criterion for choosing elemental compositions that may result in rocksalt structure (B1) high-entropy ceramics with improved plasticity: valence electron concentration (VEC) >9.5 e-/formula unit to populate bonding metallic states at the Fermi level (reduced brittleness). Here, single-phase B1 (HfTaTiWZr)C and (MoNbTaVW)C are synthesised and tested as representative systems due to their unique VEC values. According to statistical analysis of nanoindentation arrays at different loads and depths, (HfTaTiWZr)C (VEC=8.6 e- /f.u.) is hard but brittle, whereas (MoNbTaVW)C (VEC=9.4 e- /f.u.) is hard and significantly more fracture-resistant than (HfTaTiWZr)C. The improved fracture-resistance of (MoNbTaVW)C under deformation may result from the intrinsic material's capacity to undergo local lattice transformations beyond tensile yield points as well as from relatively simple activation of lattice slip, according to *ab initio* molecular dynamics simulations and electronic-structure analysis. Additional simulations, done to track the evolution of mechanical properties as a function of temperature, predict that (HfTaTiWZr)C will stay brittle at all tested temperatures, although (MoNbTaVW)C may maintain good resistance to fracture up to 900 K–1200 K.

Keywords: *High-entropy ceramics; Ab initio molecular dynamics; Stress-induced transformation; Fracture toughness; Nanoindentation; Valence electron concentration*

Introduction

High-entropy alloys are a fast growing topic, and as a result, innovative material systems with exceptional or novel features have recently been developed. The idea of configurational entropy stabilization and investigation of compositionally complicated solid

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solutions has been applied to ceramics, continuing the trend of high entropy alloys, making it feasible to uncover realistic compositions that were previously thought to be impossible. The first entropy-stabilized oxide, a rock salt (B1) structured (MgCoNiCuZn), was described by Rost et al. and showed that a single phase can form above a critical temperature [1]. Numerous reports on high-entropy ceramics, such as oxides, borides, carbides, nitrides, carbonitrides, and silicides, have been published since this first work. Due to its numerous desirable qualities, such as high melting temperatures and high-temperature mechanical stability, High-Entropy Carbides (HEC) are plausible candidates for ultra-high temperature applications, such as hypersonic flight leading edges and high temperature reactor linings [2]. In addition to better creep resistance, good oxidation resistance, low thermal conductivity, and great resistance to radiation damage, HEC has shown higher hardness compared to their expected rule of mixtures values. High flexural strength of 421 MPa has been observed in the high-entropy carbide (HfNbTaTiZr) C, which is sustained until 1800 C and drops to 318 MPa at 2000 C [3]. The high degree of randomness and lattice aberrations that are specific to high-entropy materials are thought to be the cause of the high hardness. The potential usage of ceramics is severely constrained by the fact that high hardness (which is connected to high mechanical strength in solids) is frequently insufficient to prevent brittle fracture [4]. In fact, a monolithic solid ceramic phase typically is unable to combine high strength and great fracture resistance, which correlates to superior toughness [5].

Discussion

Nanoindentation reveal that (MoNbTaVW) is significantly more resistant to fracture than (HfTaTiWZr). Uniaxial tensile deformation modelled via AIMD for pristine crystal models can help to explain the variations in observed response of (HfTaTiWZr) and (MoNbTaVW) under indentation load because the stress field generated under a Berkovich indenter includes tensile stresses at the indenter corners, where radial (Palmqvist) fracture occurs [6]. By altering the bonding network at the fracture front, the changes brought on by tensile elongation in (MoNbTaVW) C may prevent crack formation and/or propagation. Additionally, the results of AIMD demonstrate that lattice slip in (MoNbTaVW) C is activated at lower shear stresses than in (HfTaTiWZr). The ideal (MoNbTaVW)C crystals' considerably lower lattice slip resistance and easier stacking fault development may open up new channels for stress dissipation at the crack tip (i.e., enhanced plasticity) [7,9]. The desired lattice structure of binary elements and the alloy's electron concentration are crucial design factors for high-entropy ceramics with improved hardness and toughness, as will be covered below. Due of their unique VEC values, (HfTaTiWZr) C and (MoNbTaVW) C are chosen as exemplary high-entropy carbide systems in this work. It is anticipated that (HfTaTiWZr) C will have extremely high hardness due to its electron concentration. The VEC of (MoNbTaVW) C, in contrast, is ideal for producing a material with high hardness and enhanced plasticity pathways that may eventually result in higher toughness [8,10].

Conclusion

Experiments and AIMD simulations were used to study the mechanical behaviour of high-entropy carbides. The two compositions, (HfNbTaTiZr) and (MoNbTaVW), were selected to show distinct differences in flexibility and resistance to fracture, with valence electron concentrations of 8.6 e-/f.u. and 9.4 e-/f.u., respectively. Experimental fracture frequency measurements in indentation arrays at various pressures and depths show that (MoNbTaVW), which is more electron-rich, has greater fracture resistance than (HfNbTiZr). While indents into the (MoNbTaVW)C sample consistently do not display fracture up to 500 mN force, all indentations into the (HfNbTaTiZr)C sample fracture with as little as 250 mN force (or 600 nm depth) (or 1,000 nm depth). To support the observed variations in ductility and fracture resistance, defect free supercell models' tensile deformation along the crystal axes was simulated using AIMD. These findings suggest that changes in the bonding network brought on by the material yield point may be the cause of the higher resistance to fracture in (MoNbTaVW) C. Depending on the loading direction, the transformation toughening mechanisms for pristine (MoNbTaVW) C that have undergone tensile strain involve a loss in atomic coordination. For instance, the sixfold-coordinated

B1 lattice locally converts to a fivefold-coordinated graphite-like structure when subjected to elongation. Additionally, the AIMD simulations demonstrate that the energetic preference to form stacking faults is enabled by the d-d electron hybridization activated with shear deformation in carbide with VEC 9 e- /f.u. This energetic preference may enable additional stress dissipation at crack tips through the creation of new plasticity routes, positively influencing the material's resistance to fracture [10].

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