
Tailoring Mechanical Properties and Deformation Behavior in amorphous/crystalline Zr40Cu60/Fe Nanolaminates

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Abstract

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Amorphous/crystalline nanolaminates are known for their tailored mechanical properties by adjusting the microstructure, density of interfaces, and bilayer period (L), leading to large yield strength and plasticity (1). For instance, in amorphous/crystalline CuZr/Cu nanolaminates, tuning the thickness of the amorphous layer leads to enhanced plasticity by suppressing shear band instability, achieving a maximum tensile strength of 2.5 GPa and $\approx 4\%$ strain at failure (2). Similarly, adjusting the crystalline layer thickness can suppress the catastrophic propagation of shear bands by promoting a homogeneous deformation and achieving a yield strength of 2.6 GPa and plasticity of 40% in compression (3).

However, critical questions remain regarding the effect of amorphous/crystalline interfaces on the mechanical properties and how they affect the deformation mechanisms (2). In addition, it is critical to gain insight into the critical layer thickness required to initiate plasticity and effectively suppress shear band formation, as well as to understand the deformation mechanisms in the amorphous/crystalline nanolaminates (1). Moreover, the use of BCC crystalline layers remains less explored.

In this study, we synthesized $2\mu\text{m}$ -thick Zr40Cu60/Fe-BCC nanolaminates by magnetron co-sputtering. Nanocrystalline Fe has been selected for its high mechanical resistance and positive mixing enthalpy with Cu, which limits intermixing, to form well-defined interfaces to block shear band propagation effectively. First, we varied the Zr40Cu60 layer thickness (from 10 up to 90 nm), keeping the Fe layer equal to 10 nm, to investigate the transition from localized plastic to homogeneous deformation in the amorphous layer. In a second approach, we kept the same volume fraction of Zr40Cu60 and Fe layers, varying the bilayer period (L), from 20 up to 80 nm, effectively tuning the density of interfaces ($2/L$). The atomic and microstructure have been investigated by transmission electron microscopy and x-ray diffraction. Optoacoustic techniques, nanoindentation, and in-situ micropillar compression

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tests were carried out to achieve a complete understanding of their mechanical properties under different loading conditions.

Regardless of the architecture, the elastic modulus of the nanolaminates closely follows rule-of-mixture predictions (2), while the hardness is significantly higher than that of the individual layers. Notably, the hardness increases with higher interface densities, reaching 9.6 GPa in the 10/10 nm Zr₄₀Cu₆₀/Fe nanolaminate ($2/L = 0.1 \text{ nm}^{-1}$) due to shear bands blocking at the interfaces and dislocation pile-up. In-situ micropillar compression tests reveal that nanolaminates with 90 nm Zr₄₀Cu₆₀ layers undergo localized deformation with percolative shear bands similar to monolithic Zr₄₀Cu₆₀. In contrast, nanolaminates with thinner Zr₄₀Cu₆₀ layers exhibit delayed shear band propagation and achieve yield strengths of up to 2.5 GPa. Nanolaminates with a 40 nm bilayer period demonstrate a delocalized shear band distribution effectively blocked by Fe layers, enabling compressive plastic deformation up to 45% and a yield strength of 2 GPa.

These findings highlight the potential of amorphous/BCC-crystalline Zr₄₀Cu₆₀/Fe nanolaminates as high-performance materials, offering tailored mechanical properties and a unique combination of exceptional strength and plasticity.

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