Tailoring composition and microstructure to control mechanical properties and thermal stability of thin film metallic glasses

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Abstract

Thin film metallic glasses (TFMGs), with thicknesses below _˜500 nm, are materials characterized by a unique mechanical properties involving large yield strength (close to the theoretical limit) and ductility (> 10%) due to the activation of mechanical size effects (1). However, several scientific questions dealing with their mechanical properties and deformation behavior together with thermal stability are still open, especially focusing on the role of the composition, addressing key questions involving the effect of local order, bond strength and free volume. This is crucial in order to synthetize TFMGs with engineered microstructure (i.e. fully amorphous nanolaminates) with even controlled/boosted mechanical properties and high thermal stability which can be maintained and extended to large thicknesses (> 3 um).
Within this context, I will first focus on the effect of composition on mechanical and thermal properties of ZrxCu100-x TFMGs with a large composition range from 24 up to 61 Zr at.% (2). Different crystallization temperatures have been found with the maximum value of _˜380∘C for Zr52Cu48, reporting the highest number of mixed Zr-Cu bonds and mixing enthalpy. Moreover, the hardness increases with Cu content, from 5.5 up to 7.7 GPa for Cu-rich specimens showing a closer atomic distances and stronger bonds. Additionally, the loading rate dependency analysis revealed that larger pop-in's appeared at low Cu (at.%) content due to a more disordered atomic structure with less strong atomic bonds enabling the formation of annular shear bands around the indent (2).

In a second part of the talk, I will expand the TFMGs compositional space to ternary alloys in which Al is added to ZrCu (from 0 to 12 at.%), while focusing on the mechanical properties and thermal stability (3). Synchrotron X-Ray diffraction reveals that the addition of Al reduces the average interatomic distances by _˜10 pm with the formation of shorter bonds (Al-Zr and Al-Cu), influencing the mechanical response (shear/elastic moduli and hardness) which increases by _˜15% for 12 at.% Al. The glass transition (Tg) and crystallization (Tx) temperatures increase by Al addition reaching 450 and 500 ∘C, respectively, for ZrCuAl12 due to the reduction in atomic mobility inhibiting atomic reconfiguration (3).

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Finally, I will show how we can exploit the previous knowledge with the fabrication of fully amorphous Zr24Cu76/Zr61Cu39 and ZrCu/ZrCuAl9 nanolaminates with different nanoscale bilayer period (from 200 down to 50 nm) and total thickness of 3 um (4). The combined effect of local chemistry variation and nanointerface density influences the thermal stability as well as the deformation behavior and the mechanical properties with severe shear displacements and strong compositional intermixing along the shear band-deformed zone. Among the main results, I will show an enhanced thermal stability above the single layer constituents as well as modular mechanical properties with large plastic deformation ($>$ 10%) in compression together with yield strength values $>$ 1.5 GPa achieved for the smallest bilayer periods.

In conclusion, I will provide guidelines to the design of compositional and microstructural-tailored TFMGs with tuned mechanical properties and thermal stability with potential impact for applications.

References:

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