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Revealing the structure and composition of small interfacial volumes composed within reactive multilayer thin films

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The nature of thin interfacial volumes (complexions) that form within vapor-deposited multilayers impact overall film function and application, yet, little is often known about the physical structure and chemical makeup of these nanometer-scale thick regions. For example, atomic species deposited as part of a multilayer can mix across interfaces leading to a modified compositional profile that affects a vital material characteristic such as thermal conductivity or stored chemical energy. With this presentation, we describe the chemical arrangement and phase of thin interfacial volumes developed in reactive Al/Pt and Co/Al multilayers and highlight their impact on film performance. Both sputter-deposited multilayers develop nanoscale, blended volumes at metal/metal interfaces as a result of favorable alloying thermodynamics. The thickness of these mixed volumes are ~15 nm and 5 nm, respectively. Portions of the intermixed Al-Pt and Al-Co volumes are amorphous. Aberration-corrected transmission electron microscopy (TEM) and energy dispersive spectroscopy (EDS) are used to further determine the compositional profiles within the blended regions. Application of a thickness-resolved Cliff-Lorimer K factor enabled mapping of nanoscale compositional variations through thickness. Direct comparisons of composition maps to complimentary, high-resolution TEM images also pinpoint a range of composition that is associated with the development of an amorphous structure. In particular, amorphous Al_xPt_{1-x} is formed over a range of Al-rich composition from x = 0.4 to 0.8 consistent with the previous, ion-beam analysis by Blanpain et al. (Phys. Rev. B 39, 13067). Lastly, we present results from complimentary Molecular Dynamics (MD) simulations that investigate the stability of amorphous atomic structures developed in binary metal systems. MD simulations were used to melt and quench model Al_xPt_{1-x} alloys of various fixed composition to obtain relaxed, but heavily disordered, structures like those observed by experiment. The MD simulations generally confirm a stable, amorphous bimetal structure in Al-rich Al_xPt_{1-x}. The predicted compositional range of amorphous Al_xPt_{1-x} and that estimated from TEM/EDS have been verified by separate control experiments that co-deposit blended alloy thin films of different uniform composition.

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