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Abstract for an Invited Paper
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On the atomic-scale design of metal-metal heterointerfaces¹

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I will describe a multiscale modeling effort to understand and control the properties of heterointerfaces in metal-metal nanocomposites, using their effect on radiation response as an example. For selected model interfaces, atomistic simulations are used to characterize interface structure and to determine the mechanisms of interface-point defects interactions, including trapping, diffusion, and defect reactions. This information is then incorporated into mesoscale dislocation-based and continuum approaches to investigate the steady-state interface response to radiation-induced defect fluxes. With insights gained from studying this “forward” problem of predicting radiation response of selected model interfaces, one may attempt to solve the “inverse” problem of determining what interfaces will yield desired radiation response.

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