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Design of composite materials for outgassing of implanted He

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We demonstrate the computational design of solid-state interfaces patterned to achieve templated precipitation of implanted helium (He). By combining multiscale modelling with designer experiments, we show that at fcc-bcc interfaces, He initially precipitates into a quasi-periodic array of stable, sub-nanometer platelet-shaped clusters. This behavior is due to the spatial heterogeneity of interface energy: He wets high energy, “heliophilic” regions while avoiding low energy, “heliophobic” ones. At semicoherent interfaces, the heliophilic regions are located at misfit dislocation intersections (MDIs).

We then develop a set of criteria that MDI distributions must satisfy to promote the precipitation of He into stable linear channels, rather than isolated precipitates, and identify several candidate heterophase interfaces whose MDI distributions satisfy these criteria. Such channels are pathways for the removal of He through outgassing and may be used to mitigate He-induced damage in future structural materials in nuclear energy applications. Our design ensures robustness by providing solution envelopes, rather than discrete optimal solutions, and incorporates synthesis as a constraint.

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