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Atomistic simulation of interfaces in glass/crystal composites for nuclear waste forms

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High-Level Waste (HLW) resulting from fuel reprocessing is immobilised in a borosilicate glass matrix, particularly in France and the UK.

Some HLW components have higher melting points than the glass, and thus never dissolve into the melt.

Other crystalline phases may also form during fabrication due to limited solubility.

Separation could also occur later through a process of devitrification.

The resultant waste form may therefore demonstrate significant heterogeneity with secondary crystal phases embedded in a glass matrix.

The purpose of this study is to improve understanding of the issues associated with such microstructures in vitrified wasteforms.

We will present results from atomistic simulations showing properties of glass/crystal interfaces in a surrogate composite formed of $(\text{Na}_2)_x(\text{SiO}_2)_{1-x}$ glass and rutile TiO_2 crystals.

The potentials employed have been widely used for glass materials. We will discuss their applicability to glass/crystal composite structures.

We will show structural and energetic features predicted for these interfaces and consider the effect of radiation damage.

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