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Atomistic simulations of silver diffusion within a titanium nitride matrix

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To mitigate the carbon footprint of aerospace industry, light and high-performance materials are currently needed, however they are very difficult to cut and machine. Self-lubricating coatings represent a way to reduce the wear of machining and cutting tools, hence increasing their lifetimes with clear advantages in terms of environmental sustainability. In this sense, it has been recently shown that TiSiN(Ag) nanocomposite coatings are very promising.[1,2]
In such systems, the diffusion rate of silver within the matrix plays a critical role and needs to be fully understood and controlled.
Here we apply both density functional theory (DFT) calculations and classical molecular dynamics (MD) simulations to gain insight into the transport of silver within TiSiN coatings. The formation energies of defects such as Ag interstitials and substitutions have been obtained with DFT. Bulk TiN, TiN GBs and at the TiN/SiN monolayer interfaces have been considered. Potential energy landscapes were obtained for the diffusion of Ag atoms on free TiN surfaces, as well as along Duffy-Tasker and Kingery type TiN grain boundaries.
MD simulations of TiN/Ag systems to observe the silver diffusion in presence of GBs and surfaces at different temperature and pressure conditions, for which a hybrid MEAM/Mie force field has been developed.[3]
Our results indicate that the diffusion along TiN surface is the fastest diffusion mechanism. Diffusion along grain boundaries is slower and directly related to the size of GB. On the contrary, bulk diffusion appear extremely slow, because of the high formation energy of related defects. Our study provide a clear understanding of the Ag diffusion mechanism in TiSiN/Ag coatings, indicating that the most relevant process is surface diffusion along intergranular space. Hence, acting on this process is the key to tune and improve the coating's performance.

Scientific Area

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