Atomistic simulations of silver diffusion within a titanium nitride matrix

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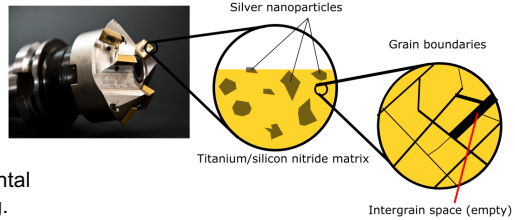
NANOTECHNOLOGIES

Background

Self-lubricating nanocomposite coatings can reduce wear of machining tools.

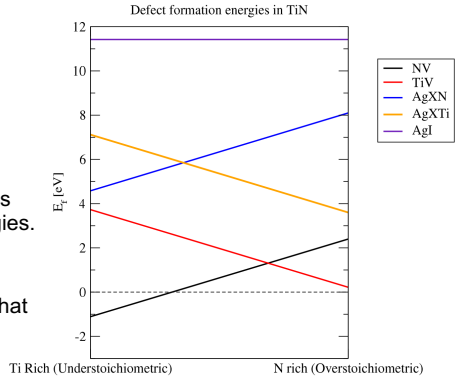
Silver is the lubricant: knowing how it diffuses across the matrix is fundamental for coating design/performance tuning.



Results

DFT calculations indicate that bulk diffusion is prevented by high Ag-defect formation energies.

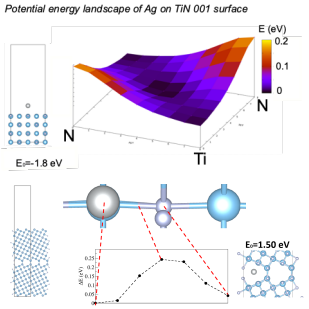
Molecular dynamics results show that Ag can diffuse along grain boundaries, and that surface diffusion is the fastest process.



Methodology

Density functional theory was applied to investigate the adsorption energy of Ag on TiN and the silver diffusion energy barriers along grain boundaries.

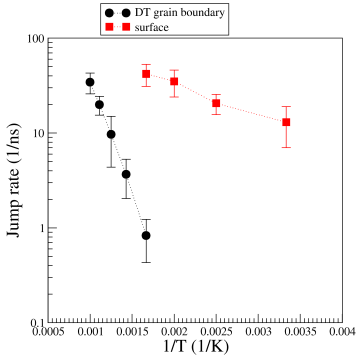
Based upon DFT, a classical molecular dynamics forcefield has been introduced to simulate large TiN+Ag systems and investigate Ag diffusion under typical device conditions.



Conclusions/Impact

We clarified the role of the different diffusion mechanisms of Ag in TiN. Our results indicate that the best way to control Ag diffusion is to act on the surface process.

Further modelling studies will address Ti/SiN+Ag systems.



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