CONTROLLUB

Self lubricant coatings for high temperature applications with controlled released of the lubricious agent

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NANOTECHNOLOGIES

Background

Self-lubricant coating systems with release of the lubricous species have enormous potential to be used in the protection of surfaces of components working in extreme conditions of wear. However, the rapid release of the lubricious agent and, consequently, its total depletion from the coating has delayed the transfer of these coatings to the industry, not being still an alternative to existing solutions. This project was focused on the development of a new class of thin films with capacity to control the lubricious metal release, in order to get a proper long term solid lubrication at high temperature conditions.
Nanocomposite TiSiN films composed by nanograins of TiN imbibed in a Si-N matrix was the solution proposed to control the lubricious Ag ions to reach long term lubrication. In fact, Si-N phase is well known to have anti-diffusion properties which, if proper tailored (thickness and distribution), can control the lubricious agent release. Therefore, projects idea was to explore the benefits of this nanocomposite structure with high dense interfaces as a tool to control the diffusion of silver (Ag) which we want to use as lubricious agent at high temperatures. A proposed synergy between atomistic simulations with experimental research was implemented for the success of the work plan.

Approach/Methodology

The core objective of this project was the development of a class of thin films with capacity to control the lubricious metal release, in order to reach long-term solid lubrication. We tailor the structure of the TiSiN films (i.e. thickness of a (quasi)amorphous SiNx matrix and TiN grain sizes) to delay the release of Ag to the surface coating by playing with the main relevant parameters of a new technology, HiPIMS – high power impulse magnetron sputtering. Progressive increase of Ag concentration on the mechanical properties, structure, physical properties, oxidation, thermal stability and tribological performance was extensively evaluated. The diffusion processes occurring during coatings annealing/oxidation were deeply studied by scanning electron microscopy and TEM transmission electron microscopy to understand the diffusion rates and diffusion paths for Ag. Atomistic simulations of the defect structure in TiN and TiSiN materials were performed, within the density functional theory, to understand the main Ag diffusion mechanism in these materials and get further insight on the experimental observations of Ag transport paths in TiN related materials.

Implementation Challenges

The main challenge faced by this project was related to the hiring of the researchers planned to work at 100% at the different partners (University of Coimbra and University of Minho). At the University of Coimbra, it was possible to contract the researcher almost at the end of the project and at the University of Minho such hiring was not even possible, due to the fact that no applications were received in successive calls for the BIPD grant. In fact, current legislative framework has further restricted the granting of this type of BIPD scholarships, making it impossible to hire human resources trained in the Research Unit and or PhDs with post-doctoral experience over 3 years, thus reducing drastically the number of eligible and interested candidates. Due to this fact, the scientific execution has been currently ensured by endogenous human resources, whose dedication has been limited. An extension of the project was thus asked in October 2019 to help in the scientific execution of the project. The COVID-19 pandemic introduced extra limitations to scientific execution with the closure of most of the research and academic institutions in Portugal and US.
Regarding the experimental analysis, we found some challenges to prepare the thin film foils for TEM observations. This preparation was very difficult and different steps between TEM analysis and further thinner of foils in FIB were required for proper analysis. Second, simple three-layers stack films initially predicted to study the diffusion of Ag, and validate simulations of Ag diffusion, failed when submitted to high temperature. Arquitecture of stacks layers needed to be re-defined, which will provide essential validation data for Ag diffusion mechanisms. Concerning, the simulation of Ag diffusion it was planned initially to use molecular dynamics to obtain quantitative values for diffusion coefficients of silver in the bulk TiSIN materials, however, the existent forcefield for TiN revealed some flaws preventing the reliable simulation of Ag diffusion in TiN based materials. In alternative, we opted to use density functional theory to get further insight into the main mechanisms governing Ag diffusion in TiSIN.

Main Findings

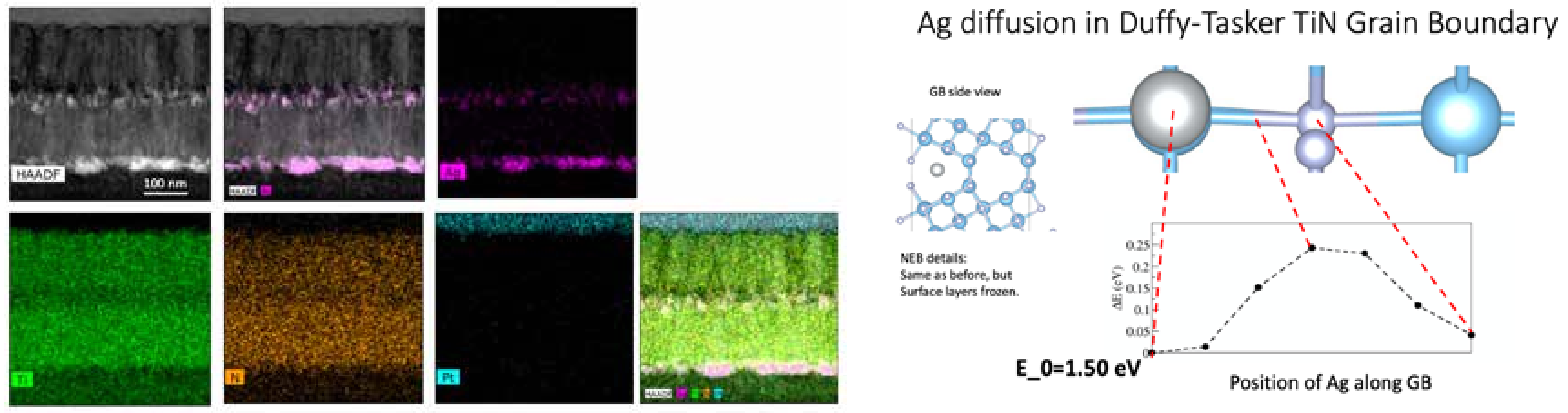
We found out that the TiSiN system deposited as nanocomposite structure allows to effectively control the lubricious element diffusion to the surface, allowing to reach long term lubrication during high temperature service conditions. We also proved by tribological testing that Ag allows to decrease the friction coefficient values at high temperature conditions and reduce the amount of adhered material from the ball to the coating surface which, from a machining perspective, is an interesting result since it helps prevent one of the most common failures of tools when machining titanium alloys, which is the formation of built-up edges. Preliminarily machining tests revealed that newly developed TiSiAgN films outperform "tested" industrial solutions available at the market to machine Ti alloys for certain machining conditions.
We were able to uncover the main mechanisms governing Ag transport in TiN based materials. Ag diffusion in bulk TiN is mediated by vacancy in Ti and nitrogen sub-lattices, with N vacancy being the most probable defect and not by the occupation of interstitial positions. We also found that the energy barrier for Ag diffusion in Duffy-Tasker grain-boundary is only 0.2 eV, revealing that Ag diffusion in GB is very fast compared to diffusion in bulk.

Expected Impact

The new developed films will impact the scientific and industrial community. It is expected that newly developed film will revolutionize manufacturing by providing additional functionality, increase lifetime and reliability of components for several industries (e.g. machining, stamping, forming, automotive, aerospatial), while reducing energy consumption, CO2 emissions, maintenance and avoiding of the use of hazards lubricants, having, thus, direct impact on society and economy. New breakthrough in simulation aspects, deposition technologies and films will allow advanced knowledge beyond the present state of the art.
In a short term, it will contribute to considerable increase to the groups and host institutions international recognition, allowing new collaborations to be established at national and international level and exploiting its scientific and technological outcomes in follow up projects and PhD/Post-Doc programs.
In fact, outcomes of this project already allowed to propose a new industrial project with current academic institutions which was recently approved for funding: Project MCTool21 - Manufacturing of cutting tools for the 21st century: from nanoscale material design to numerical process simulation, ref. "POCI-01-0247-FEDER-045940".

Project Highlights

- Newly self-lubricant coatings with proper control release of the lubricious phase which can provide long-term lubrication at high temperature were successfully produced.
- Deposition of hard and dense nanocomposite Ti-Si-N(Ag) films by high power impulse magnetron sputtering working in deep oscillation mode without the need for energetic bombardment.
- The main mechanisms governing Ag diffusion in bulk TISiN materials were uncovered, with silver transport being mediated by vacancy and not interstitial defects.
- The energy barrier for Ag diffusion in Duffy-Tasker Grain boundaries is as low as 0.2 eV, supporting the evidence of GBs as one main paths for Ag diffusion in TiN.
- Corrected forcefield for molecular dynamics simulation of TiN:Ag based materials.



Elemental STEM/EDS maps the distribution of a TiN/TiN(Ag)/TiN stack layer annealed at 800 ºC for two hours showing the diffusion of Ag and the path on TiN layers.

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