## **Microstructure and Related Properties of Nanocomposites for Tribomedical Applications**

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It has recently been established that nanocomposite thin films are promising materials for applications as wear-resistant protective coatings [1-3]. These films consist of two or more nanocrystals embedded in an amorphous or nanocrystalline matrix. When optimized, the mechanical and tribological properties of these structures are far superior to their constituent phases. First, these materials are harder due to the hindering of dislocation motion at interfaces. Second, they are tougher since their architecture favors the hindering of crack development and propagation and enhances ductility by grain boundary sliding [4]. Finally, their properties may be tailored by selecting appropriate phases and volume fractions for specific applications.

 $ZrN/M$  (where  $M = Ag$ , Au, or Pd) thin films were prepared by unbalanced magnetron DC sputtering on polished Si (100) wafers. The list of prepared samples and the corresponding deposition conditions for the ZrN/Ag system are listed in Table 1. This material was selected because of its superior mechanical properties compared to the ZrN/Au and ZrN/Pd sytems. The structure of zirconium nitride as determined by X-ray diffraction changed substantially with the addition of M as shown in Fig. 1 for the ZrN/Ag system. These observations suggest that the deposits consisted of a nanocomposite structure that comprised separate ZrN and Ag phases. Bright field TEM micrographs for sample S2 containing 12 % Ag (Fig. 2) illustrated nanometric Ag precipitates (dark particles) embedded in a ZrN matrix (light). The atomic concentrations of Ag, Zr, and N were estimated using the areas under the Ag<sub>3d</sub>, Zr<sub>3d</sub>, and N<sub>1s</sub> peaks of the detected X-Ray Photoelectron Spectra, and the silver content is summarized in Table 1. Figure 3 shows the ZrN/Ag deposit hardness and elastic modulus as a function of silver content. The hardness of the deposit increased gradually with the increase in Ag content to a maximum value of 32 GPa when Ag content reached 12%. Further addition of Ag resulted in a decrease of hardness. Figure 4 shows the  $H^3/E^2$  ratio as a function of silver content. This ratio reflects the resistance of material to plastic deformation during contact events [2]. The highest  $H^3/E^2$  ratio is obtained for sample S2. The resistance to plastic deformation was optimized for the three sets of materials and was found to depend on the choice of the metallic element (Ag being the best). These findings were attributed to the bonding mechanism at the interface between the ceramic nanocrystals and the metallic matrix as shown using ab-initio calculations using density functional theory calculations.

## References

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**Figure 1:** XRD spectra of ZrN/Ag films.



**Figure 2**: Bright field TEM image for sample S2. **Figure 3:** Hardness and elastic modulus.



Samp.	<b>Silver Target</b>	Substrate	Ag content
	Power $(W)$	Voltage (V)	from XPS (%
		$-70$	
		$-70$	$12\pm1$
S <sub>3</sub>		$-70$	$20 \pm 1$
		$-70$	$41\pm1$
S5	13	$-70$	$58 \pm 1$
	18	-70	$83 \pm 1$

Table 1: Deposition conditions and silver content for sputtered ZrN/Ag films.



 $/E^2$  values.