## Design of Novel Graded Microstructures for Cutting Tools Assisted by High Resolution Microscopy and Thermodynamic Modeling

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The design of cutting materials includes the definition of their composition and manufacturing process to produce microstructures with tailor-made properties. In this work results on recent studies for the design of interfaces and gradients in Fe-Ni-Co based cemented carbides and Ti(C,N)-Al2O3 wear resistant coatings for the production of novel cutting tools are presented. Experimental conditions for the production of graded microstructures on cemented carbides and coatings are defined considering thermodynamic factors, the use of computational thermodynamic and kinetic modeling (CALPHAD method) and high resolution characterization tehcniques.

The formation of gamma-phase-free layers on hardmetals with Fe-Ni-Co binders was studied and experimental correlations between binder composition and gamma-phase-free layer thicknesses were found [1]. Gamma-phase-free layer growth kinetics is enhanced by addition of Fe to Co and Ni binders, which is mainly promoted by the higher N solubility in Fe compared to Co and Ni binders. Thermodynamic calculations of N solubility in the liquid binder phase showed good correlation with layer thickness growth kinetics, showing that Fe-containing binders promote the formation of thicker gamma-phase-free surface layers.

The influence of Fe-Ni-Co binder composition on nitridation of cemented carbides with Fe-Ni-co binders was also investigated [2]. It was found that the nitrided zone formation obeys a parabolic law (diffusion-controlled process). The thickness of nitrided zone is larger for cemented carbides with Fe-based binders, due to larger N solubility in Fe but also enhanced diffusivity of N in Fe containing binders. The kinetics of nitrided zone formation is controlled by N diffusion in binder phase. Thermodynamic calculations of N solubility levels in Fe-Ni-Co binders showed good correlation with layer thickness growth. The influence of nitridation on surface microstructure and properties of graded cemented carbides with Co and Ni binders was studied by HR-TEM and XRD [3]. TEM observation of defects and morphology in Co and Ni binder phase by TEM showed stacking faults for the Co binder and twins for the Ni binder. Rietveld refinements of XRD was applied to study domain size and microstrain in nitrided zone, showing significant reduction of the carbonitride grain size in the nitride zone. The formation of the nitride zones was found to be correlated to preferred dissolution of core-rim structure in presence of N atmosphere. Nitrided cemented carbides presented enhanced tool performance compared to standard non-graded cemented carbides.

The production and characterization of novel wear resistant Ti(C,N) coatings manufactured by modified chemical vapor deposition process was investigated [4]. Ti(C,N) coating layers produced by a modified HT-CVD method allows to control the C/N ratio of Ti(C,N) layers by the deposition conditions. Star-shaped and lenticular-like Ti(C,N) crystallites form the mod-HT-CVD layer. Ti(C,N) layer formation investigated by interrupting the mod-HT-CVD process. Mod-HT-CVD Ti(C,N) layers presented higher wear resistance than MT-CVD layers. Furthermore the synthesis of titanium carbonitride coating layers with star-shaped crystallites produced by modified CVD. It was observed that the

5-fold symmetry retained to produce large star-shaped particles of 500-600 nm. TEM studies showed that the mismatch in pentagonal structure accommodated by formation of SAG boundary of  $6.4^{\circ}$  and that the distortion of the tetrahedra for further elastic stress relaxation of crystallites. The novel Ti(C,N) coatings manufactured by modified chemical vapor deposition were combined with a Al2O3 top layer coating for the design of novel wear resistant multilayer CVD coatings with improved adhesion between Al2O3 and Ti(C,N) [6]. One fundamental microstructure feature to improve the adhesion of the layers was the design of graded Ti(C,N) layer with needle-like transition to the Al2O3 layer. 3-D FIB tomography study of Ti(C,N) grains and interface Ti(C,N)-Al2O3 layer was carried out showing a interlocking bonding between layer. The improved adhesion of the Al2O3 layer enhances the performance of the cutting tools considerably.

Finally the role of cemented carbide graded outer-layer formation on the wear performance of coated cutting tools was investigated by combining both the graded cemented carbides and the novel graded CVD coatings [7]. Comparison of cutting performance of coated tools with functionally graded substrates was carried out. Gamma-phase enriched-surface layers improve tool life in finishing operations. The main effect of fcc-rich layers is retardation of crater wear and plastic deformation. Gamma-phase-free layers present stable cutting tip performance in interrupted cutting. Wear response of Ti(C,N)-Al2O3 multilayers improved by interlocking effect due to graded transition of the layers.

Summarizing this work shows how the interaction between experimental work, thermodynamic modeling, kinetic simulation and high-resolution characterization can be applied to produce new microstructures in modern hard metals.

References:

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Figure 1. Interlocking effect of the novel HT-TiCN – Al2O3 top layer [6].