Thursday Afternoon, April 26, 2018

Special Interest Talk 2
Room San Diego - Session SIT2

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4:10pm **SIT2-9 Materials Design Guidelines for Improved Strength, Ductility, and Stability***, **Paul Heinz Mayrhofer**,* TU Wien, Institute of Materials Science and Technology, Austria

Whenever mechanical attack is dominating the loading profile of materials in industrial applications, nitrides are highly preferred, whereas oxide materials provide best protection against high temperature corrosions. Thus, when mechanical and thermal loading is combined, the nitrides used should also provide an excellent stability against temperature as well as corrosive attack (such as oxidation). How nitride materials can be developed – implementing computational and experimental materials science – to withstand high mechanical as well as thermal loading, is the focus of this talk.

We will use recent developments – where we applied alloying and architecture concepts (e.g., composition and/or phase modulated layers) to transition metal nitrides, for optimizing their properties – to derive important materials design guidelines for improved strength, ductility, but also stability. Especially the stability (here, we concentrate on phase stability with respect to chemistry and temperature, but also on the stability against oxidation) of nitrides is an extremely interesting task, as for example the face centered cubic (fcc) structure of TiN_x is rather insensitive to small (or even large) variations in chemistry and alloying elements (TiN even allows for the substitution of 66% Ti with Al to still crystallize in the fcc structure). Contrary, the preferred crystal structure of other transition metal nitrides (like MoN_x and TaN_x) is extremely sensitive to small chemical variations, even if only the vacancy content changes. Nevertheless, especially Ta is extremely versatile in increasing strength, but also ductility, as well as the thermal stability and oxidation resistance of Ti-Al-N coatings, which are still an extremely important material class.

With the help of various superlattice coatings, we show that also with such architectural concepts, strength and ductility (here, basically obtained by in-situ micromechanical cantilever bending tests) can be improved simultaneously. Additionally, we also give an example of transformation induced plasticity mechanisms, which can be implemented in nitride materials as well.

The individual concepts will allow designing materials to meet the ever-growing demand for further improved coatings, tailor made for specific applications.

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