Mesoscale modeling of hardmetal

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ABSTRACT

WC-Co systems constitute an important class of hardmetals. On the mesoscale they consist of WCgrains in a (more or less) contiguous binder phase of Co. Clearly, a realistic topological and geometrical description of the mesoscale structure is needed in order to make the analysis meaningful. Primarily computational homogenization is used to predict the engineering properties. An important parameter for the mesoscale generation is the volume fraction of the phases (including possible rest porosity). Other characteristics are shape-, size-, and orientation-distributions of WCgrains, and the contiguity. Moreover it is necessary to identify intergrain and interphase boundaries. A particular issue related to the presence of ultrathin "wafered" Co-layers that must be modeled as a geometric interface (using a Cohesive Zone (CZ) model) on the mesoscale.

In the work by Magin and Gérard [1], CAD software is used to generate the WC-Co grainstructure; however, it fails to capture the inter-grain boundaries. In our approach we overcome this limitation by inserting grains in a discretized grid instead of a CAD description, which allows for simple manipulation of the contacting WC grains.

In the numerical examples, we combine crystal plasticity modeling of the bulk material with a CZmodel for WC-Co-interphases that allows for prediction of gradual degradation (damage) in the macroscale response. WC has HCP-crystal structure; hence, the pertinent symmetry affects elastic as well as the plastic properties. Calibration of the CZ-model is, at least in part, accomplished by atomistic simulations.



Figure 1: Example of computation: Mesostructure (left) and residual von-Mises stresses (right) after cooling from 1000°C

REFERENCES

[1] M. Magin and J.-S. Gérard, *Microstructure and morphology of hardmetals*, Proceedings of the 17th International Plansee Seminar, **3**, 2009.