EPMA European Hard Materials Group

Project proposal: Kinetic simulations in Hardmetals – Evaluation of Mobilities by Coupling Experiments and Simulations

"Kinetic"

Consortium Agreement

Issued October 2014

The Project – "Kinetic" as defined in Annex 1
The Contractors –

- Swerea KIMAB AB, Box 7047, Isafjordsgatan 28A, SE-164 07 Kista, Sweden: **SWEREA**
- KTH Royal Institute of Technology, Materials Science and Engineering Department, Brinellv. 23 S-100 44 Stockholm, Sweden: **KTH**

The Coordinator –

- The European Powder Metallurgy Association, Talbot House, 2nd Floor , Market St., Shrewsbury SY1 1LG, England: **EPMA**

The Members – Paid up corporate EPMA members funding the Project
The Participants – The Contractors and the Members

UV = unanimous vote of Members and Contractors; MV = majority vote of 2/3 members or higher

Heads

1. The Members and Contractors agree to cooperate in order to complete the Project according to Annex 1.
2. All information generated under the Project will remain confidential to the Members during the Project and for 5 years after delivery of the final written report to Members, and may only be disclosed to third parties (e.g. for dissemination purpose in PM Congress) with UV.

   For SWEREA and KTH: the contractor is obliged to publish in the usual scientific form the results of studies undertaken during performance of the project. The client gives their fundamental consent to such publication. The contractor will inform the client beforehand of any planned publication and will give them the opportunity of commenting on it within a reasonable period, at latest four (4) weeks after submission of the text intended for publication. A Member is entitled to refuse their consent to a publication if it is intended to publish company related data or, in connection with the granting of patent rights, if it is intended to publish any anticipatory information likely to constitute a bar to novelty. In such cases, the contracting parties will, without delay, seek to reach a special agreement governing the form and timing of rapid publication and taking due account of the legitimate interests of both parties.

3. The Contractors agree to not carry out the same project on "Kinetic simulations in Hardmetals – Evaluation of Mobilities by Coupling Experiments and Simulations" with organisations other than the Members until completion of the project (delivery of the final report). The aforementioned

obligation shall not apply to other entities of SWEREA and KTH other than its performing entity research groups.

4. The Members agree **to share equally the cost of the Project** (EUR 11,300). The required minimum number of Members is **four** unless the Members agree to exceed the maximum Project Fee.
5. The KTH Royal Institute of Technology agrees to become an associate Member (EUR 2,080 per year) of the EPMA once the "Kinetic" Project will have started.
6. **VAT**: The Project Fee is excluding VAT if applicable. Non UK participants do not pay VAT provided they give their VAT number to the EPMA. UK participants have to pay VAT regardless and then reclaim it.
7. The Members also undertake to provide the Contractors with the necessary materials (powders, specimen etc...) for the project. If no agreement on in-kind contribution between the industrial partners can be found or if the Consortium agrees to subcontract it internally or externally at additional costs, the EPMA will coordinate this task "Work Package 0" and charge equally each Member to cover the cost plus an administrative fee of 13%.
8. **Payment Schedule:**
   For Work Package 0: Full payment within one month of invoice if necessary.
   For "Kinetic" project:
   - **50% at the start**,
   - **50% after completion** of the "Kinetic" Project and delivery of the final report.
9. New paying members may be admitted during the Project by UV on payment of an additional reasonable premium (10%). The premium will be used to decrease the Project Fee for the Consortium Members.
10. Except for the deliverables of Annex 1, each Participant will retain the Intellectual Property for any other outcomes of the Project.
11. **Warranty**. The contractor's warranty extends solely to the use of due scientific diligence and to compliance with accepted engineering practice. The contractor does not guarantee that the desired objectives of the research and development project will be achieved.
12. **Liability**. The contractor is liable solely for wilful actions and gross negligence. Liability for proven damage is limited to the amount of the contractual sum.

All the terms of this agreement may be changed by UV, except for 4, 5,6, 11 & 12

Coordination will be undertaken by the EPMA, who will have responsibility for invoicing, day to day liaison with the Contractors and keeping Members informed. The EPMA will operate under the same confidentiality agreement as Members and the EPMA President will arbitrate any unresolved disputes.

Signatures: signed individually by all Members and Contractors

ORGANISATION:

VAT NUMBER:

NAME:

DATE:

SIGNATURE and STAMP:

Annex 1

Background

Tough graded surface zones can be formed during sintering by altering the phase composition of the surface zone by the influence of the sintering atmosphere. Such graded surface zones are important for coated hardmetals, where differences in properties between coating and hardmetal can cause cracks. The mechanism of formation of the gradient zones can be understood by diffusion simulations as shown by Gustafson and Östlund [1], who applied a thermodynamic and kinetic model and could show that the surface zone is formed due to a coupled diffusion of N and Ti. Ekroth et al. [2] used a thermodynamic database that described the equilibrium situation in their alloy system, coupled the thermodynamic description with diffusion simulations, and could reproduce the experimental information of gradient formation with simulations.

The background data that is needed for these simulations is both information on the mobilities of the elements, and knowledge of the phase equilibria in the system. The phase equilibria are determined by thermodynamic databases that are well known for many base systems, and will not be treated in the project. The simulations also require descriptions of the mobilities of the diffusing elements in the phases that are present. The transport of the elements will mainly take place in the liquid binder phase during the gradient formation. The evaluation of the mobilities in the liquid phase are thus of most interest. The mobilities in the carbide/nitride phases are also of interest. The diffusion of the metallic elements in the carbides/nitrides is very slow, and can in some cases be important for the microstructure development. Since there is very limited information on the mobilities, estimates are today applied. The effect of using different mobility values for the elements is significant, as shown in Figs.1-4, taken from ref. [3].

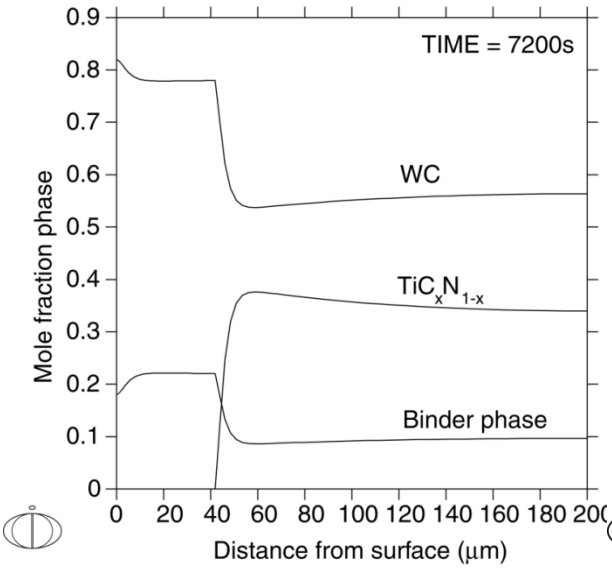

Figure 1. Simulation of gradient zone using the same mobilities for all elements.

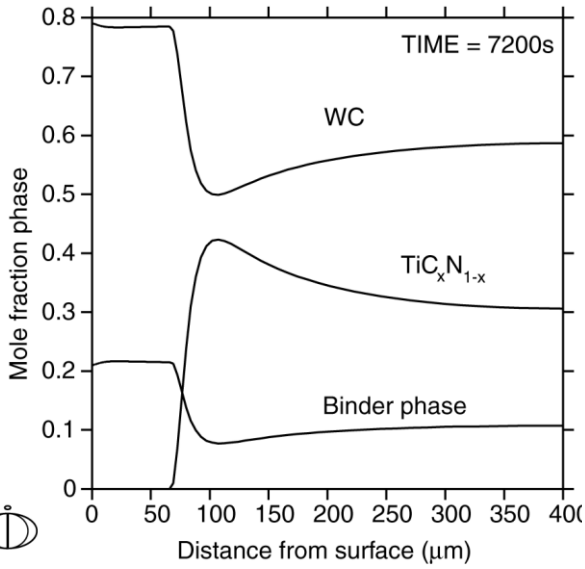

Figure 2. Mobility for N increased 10 times.

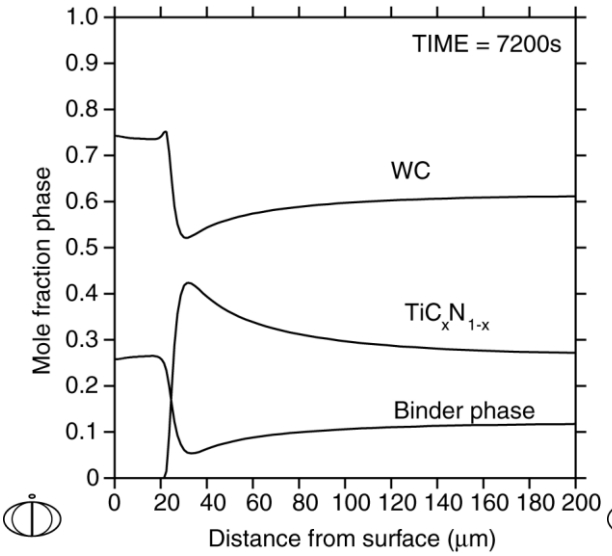

Figure 3. The mobility for the metallic elements decreased 10 times.

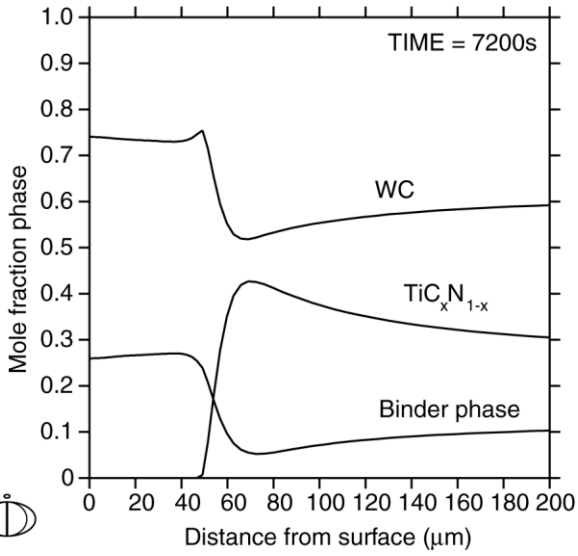

Figure 4. The mobility for the metallic elements decreased 2 times. The mobility for C and N increased 5 times.

It is very valuable to be able to accurately simulate for example the gradient formation or other phase transformations during sintering, and is thus of interest to obtain better values for the mobilities. This proposal describes a combined experimental and theoretical approach to learn more about how to determine the mobilities for a selected application to surface gradients.

1. P.Gustafson and Å.Östlund, Binder-phase enrichment by dissolution of cubic carbides. Int J Refract Met Hard Mater 1994;12(3):129–36. 2. P.Gustafson and Å.Östlund, Binder-phase enrichment by dissolution of cubic carbides. Int J Refract Met Hard Mater 1994;12(3):129.

2. Ekroth M, Frykholm R, Lindholm M, Andrén HO, Ågren J. Gradient zones in WC–Ti(C, N)–Co-based cemented carbides: experimental study and computer simulations. Acta Mater 2000;48:2177.

3.Karin Frisk, Ida Borgh, Andreas Markström, Greta Lindwall, Susanne Norgren, *Applying Computational Thermodynamic and Kinetics to Analyse the Effect of N in Hardmetals,* Proceedings of the 18th PLANSEE Seminar 2013, International Conference on Refractory Metals and Hard Materials, June 3-7 2013, Reutte, Austria, p.1215-1223. Eds: L S Sigl, H Kestler, J Wagner, PLANSEE SE, Reutte/Tyrol, Autria. www.plansee-seminar.com.

Aim

The aim of this proposal is to perform a pre-study to:

- gain a better understanding of how to select mobilities when simulating gradient formation
- evaluate possible theoretical and experimental techniques to determine mobilities
- set up a plan for further examinations

Goals/ Work plan
The work will be initiated with a feasibility study (Stage 1).

Stage 1: Feasibility study

Including to following Tasks:

1. *Literature survey:*
   The relevant experimental data will be reviewed, as well as results of simulations. Experimental and theoretical methods to evaluate mobilities will be reviewed.
   Deliverable: Report summarizing the information that is found, and highlighting the needs for further work.
   Estimated duration**: 2** months
   Distribution of tasks**:** SWEREA, KTH

2. *Selection of alloy systems:*
   The partners who will join the study will be asked to state the systems that are of interest. Based on this input, and on the results of the literature survey, a suitable alloy system will be selected.
   Deliverable: Selected alloy system for the full project.
   Estimated duration**: 1** month
   Distribution of tasks**:** Ind Partners together with SWEREA and KTH

3. *Assessment of the methods that should be used for the experiments and for the evaluation of the mobilities*
   Based on the results of the literature survey and on the selected alloy system the methods for the mobility evaluation will be selected. Discussion with possible partners to perform the experimental work will be included in this stage. For the selected system / systems the gradient formation will be simulated using DICTRA, a commercial thermodynamic database and with estimated mobilities. The effect of selecting different mobilities will be assessed and documented as a background for the further studies.
   Deliverable: Short report of the selected methods and the results of the calculations. Work plan for the stage 2.
   Estimated duration**: 3** months
   Distribution of tasks**:** SWEREA, KTH

Project Management: The work will be performed by researchers at KTH, Materials Science and Engineering Department. The project will be led by Karin Frisk from Swerea KIMAB. The EPMA will coordinate the Project.

One or two meetings and /or Conference Call with all Participants and the EPMA will be held at the beginning and/or at the end of the project.

Schedule :
Total project duration: 6 Months

Budget for project:
SWEREA: 5 000 EUR
KTH: 5 000 EUR
EPMA Management Fee: 1 300 EUR

Possible Follow up:

A possible Stage 2 will be discussed at the end of Stage 1 with the possible goals:

- experimental work
- evaluation of mobilities
- application of results to problems selected by the project group