

COST 526

**Automatic Process Optimization in Materials Technology
(APOMAT)**

Title:

A Numerically Based Optimization of a near-g TiAl Precision Casting Process

Keywords: precision casting, near g-TiAl, lamellar microstructure, heat flow, thermal expansion

Organization/Company:

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1. Duration / run time of the project

- Starting date: 1.1.2002
- Finishing date: 31.12.2004

2. Overall cost

- 110 kEURO

3. Funding situation

- Funding already assured by: Not applicable
- Funding applied for at: Not applicable
- Thinking about funding by: 1.12.2001

4. Project partners indicated to participate

- Indicate partners on national and / or European level-partners:
Department of Casting (Ass. Prof. L. Zemcik), Institute of Materials
Faculty of Mechanical Engineering, University of Technology, BRNO
Czech Republic

- Description of the collaborative approach:

Optimised parameters like the superheat of the melt, the mould temperature and cooling kinetics obtained on the basis of a numerical simulation (performed in IPM Brno) will provide a starting set of parameters for trial melts and near-net shape precision casting of near- TiAl components in the Department of Casting, UT, Brno.

- Expected mutual benefit:

Reducing the number and increasing the efficiency of expensive trial melts on the side of Department of Casting and the direct experimental verification of the numerical model prediction capability on the side of IPM are expected.

5. Project partners to be found

We are looking for the European partners who are interested in a similar type of activity, especially in the optimization of the precision casting process in general. We already have a fruitful exchange of data and conceptual ideas with our colleagues from IRC Birmingham within the framework of the COST 522 action. Looking at the recent list of projects proposed for the COST 526 action, we feel that similar beneficial collaboration could be established with projects from Germany (Dr. Laschet), Finland (Dr. Laitinen), France (Prof. Gelin) and Slovenia (Dr. Filipic).

A more difficult situation exists concerning the collaboration with industry. We are not aware of any

company in Czech Republic which would presently master the TiAl casting process, even though we were already notified of a potential interest in the future, if the trial melts prove to be viable.

6. Short description of the material process to be optimized

- Which type of process is involved:

The process to be optimised is the precision casting of the near- TiAl components like turbochargers and valves for car and aerospace engines. The optimal trade-off between processing cost, the product microstructure and quality should be found.

- Essentials of process technology:

The precision casting of high specific strength near- TiAl components is difficult for two reasons. The first issue is associated with the microstructure of the cast which must be optimised directly during the casting process since in the near-net shape technology later microstructural improvements through e.g. forging operations are excluded. The second difficulty arises due to the intrinsic brittleness of the near-TiAl alloys at lower temperatures. Rather brittle casts are prone to damage caused by different thermal expansion coefficients of the ceramic mould and the intermetallic cast. The mould strength and the cooling kinetics must be designed properly to make the technology successful and market competitive.

- Economic impact (e.g. production figures, turnover): Not specified yet

7. Material(s) involved:

- Material type of the product:

Near- TiAl alloys based on the composition Ti-48Al-2Cr-2Nb with boron addition and with controlled levels of interstitial impurities will be considered.

8. Optimization potential of the process or process step

- Quantified impact on material quality, processing time etc.:

The near- TiAl melting and casting technology in its current state is limited due to a low superheat which can be achieved when using the water-cooled Cu crucible. Moreover, the high investment cost necessary to fully commission the cold-crucible casting unit makes the process less attractive. The proposed project is thus also aimed at providing knowledge which would help to reduce the cost and improve the amount of superheat in using the standard, ceramic crucible based melting facility.

- Technological feasibility:

Recent developments in the near- TiAl casting technology indicate [1] that there is a fair chance to obtain useful products even in the case when the alloy exhibits higher content of interstitial impurities. The important prerequisite is, however, the fine microstructure of the cast.

9. Specified material properties to be achieved

- Which material qualities are to be respected or even improved:

The optimum balance between the strength and ductility could only be achieved when the near- TiAl cast possesses a fully lamellar microstructure with a controlled lamellar spacing in the range 0.1 – 1 μ m [2]. This type of microstructure represents a target attempted in the optimised precision casting process.

- What are the material defects to be avoided:

Hot-tearing and low temperature cracking of the cast parts must be avoided.

10. Process parameters to be optimized

- Identify process parameters related to material qualities or defects:

There are four process parameters which would be considered for optimisation: (i) the amount of superheat, (ii) the mould temperature, (iii) the strength and the thermal expansion coefficient of the ceramic mould and (iv) the cooling kinetics. All the four parameters are related to both, the hot tearing and the low temperature cracking of the cast. Furthermore, they also directly influence the cast microstructure which determines properties of the final product.

- What are the restraints for these parameters:

Even though the use of ceramic crucibles enables the superheat to be increased, the rate of Al depletion grows with increasing melt temperature which puts the upper limit on the superheat since the deviations from the exact alloy composition must be avoided. The mould has to be compliant enough not to cause a cast damage during cooling, on the other hand the mould must withstand the thermo-mechanical loads resulting from the casting process.

11. Material laws including material dependent coefficients

- What quantitative laws will be applied for quality function design:

The plastic relaxation of the elastic strains imposed during cooling and associated with different thermal expansion coefficients of the intermetallic cast and the ceramic mould will be based on the standard Norton law, where the rate coefficient and the stress exponent will be extracted from creep data available in the applicant's institution at present.

- Are coefficients / data available or to be determined:

Also the other necessary input parameters were already collected with the exception of a ceramic mould thermal conductivity which still needs to be determined.

12. Simulator

- Brief description of the program system to be applied for process simulation:

The software Mathematica, version 4.1 for LinuxAlpha environment will be used. The Mathematica package is open system that allows the usage of a C++ code in the critical parts of the program.

- Are there process specific software developments necessary:

Some routines will be written in the C++ code.

13. Optimizer

- Indicate optimization algorithms or software optimization environments (e.g. name of a commercial optimization software package) to be applied:

The primary concern of optimization directed to successful trial melts is to minimize the stresses build up due to different thermal expansion coefficients of the ceramic mould and the intermetallic cast. The four parameters entering the optimisation process were identified in the §10. In view of the complexity of the task we expect that, at least in the first stage of the project solution, the purely heuristic approach will be needed in which the search of the minimum will be based on the variation of one individual parameter assuming the other parameters being fixed. However, we are open to discuss this task and learn some more sophisticated approaches from our prospective partners.

14. Competence / activities of proposer:

The important background knowledge associated with the high temperature plasticity and microstructure of near- TiAl alloys has been built during the solution of two preceding projects (national project GA CR no. 106/95/1522 "Microstructural Mechanism of Creep in Advanced Materials" and international project COST 513 OC 513.10 Microstructural Mechanism of Creep in Gamma Titanium Aluminides", both of which were successfully finished in the past.

Since the year 1995, creep and microstructure of gamma TiAl have been studied in the Institute of Physics of Materials AS CR (IPM) due to the support of the two project mentioned above. It is further important to highlight that IPM has been recognised worldwide as a centre of both, competence and excellence in the field of high temperature deformation, mechanical fatigue and microstructural studies of materials. The proposed project is suitably framed within the international collaboration and activities devoted to the research of -TiAl due to IPM participating in the new action COST 522-GT WP1.2, where IPM joined with the project "Microstructure and Creep Strength of near - TiAl Alloys for Gas Turbine Applications". Mutual exchange of ideas between collaborating partners can be expected to help in successful solution of the proposed project. The applicant is also at present the principal investigator of the national grant-project GA CR no. 106/01/1590 "Impact of Alloy Chemistry and Physics on Processing and Applications of -TiAl Intermetallics".

The applicant has a long-term experience in the field of modelling of materials microstructures and processes [3-6] and leads the project "Anisotropy of Creep in Heterogeneous Microstructures" which is currently a part of the COST P3 action, project no. OC P3.50.

15. International state of the art and references

- State of the art of process modelling and optimization concerning your proposal

To the best of the applicant's knowledge, there has been no direct attempt devoted to the modelling of near- TiAl precision casting which would have been presented in the literature. However, the process itself received a considerable attention since it is the most effective processing route as far as the gas turbine components are concerned [1-2,7-10].

- Relevant publications and articles:

[1] T. Hanamura, K. Hashimoto: Ductility Improvement of Direct Cast Gamma TiAl Based Alloy Sheet, **High Temperature Ordered Intermetallic Alloys VII**, eds. C.C. Koch et al., MRS, Pittsburgh 1997, p. 71.

[2] T. Tetsui, S. Ono: Endurance and Composition and Microstructure Effects on Endurance of TiAl Used in Turbochargers, **Intermetallics 7**, 1999, 689.

[3] A. Dlouhý, M. Probst-Hein, G. Eggeler: Static Dislocation Interactions in Thin Channels between Cuboidal Particles, **Mat. Sci. Eng.**, 2000, accepted for publication.

[4] M. Probst-Hein, A. Dlouhý, G. Eggeler: Interface Dislocations in Superalloy Single Crystals, **Acta Materialia 47**, 1999, 2497-2510.

[5] M. Probst-Hein, A. Dlouhý, G. Eggeler: Superposition of External and Internal Stress Components in / '-Microstructures and Their Effect on -Channel Dislocations, **Journal de Physique IV France 9**, 1999, Pr9-127.

[6] A. Dlouhý, R. Schäublin, G. Eggeler: Transmission Electron Microscopy Contrast Simulation of <100>-type Superdislocation in L12 Ordered Structure, **Scripta Materialia 39**, 1998, 1325-1332.

[7] Y. Nishiyama, T. Miyashita, S. Isobe, T. Noda: Development of Titanium Aluminide Turbocharger Rotors, **High Temperature Aluminides and Intermetallics**, eds. S.H. Whang et al., TMS, Warrendale 1990, p. 557.

[8] D.E. Larsen: Status of Investment Cast Gamma Titanium Aluminides in the USA, **Materials Science & Engineering A 213**, 1996, 128.

[9] D. Eylon, M.M. Keller, P.E. Jones: Development of Permanent Mold Cast TiAl Automotive Valves, **Intermetallics 6**, 1998, 703.

[10] T. Noda: Application of Cast Gamma TiAl for Automobiles, **Intermetallics 6**, 1998, 709.