



# Modeling and validation of chemical vapor deposition for tungsten fiber reinforced tungsten

Leonard Raumann

Energie & Umwelt / Energy & Environment

Band / Volume 515

ISBN 978-3-95806-507-9

Forschungszentrum Jülich GmbH  
Institut für Energie- und Klimaforschung  
Plasmaphysik (IEK-4)

# **Modeling and validation of chemical vapor deposition for tungsten fiber reinforced tungsten**

Leonard Raumann

Schriften des Forschungszentrums Jülich  
Reihe Energie & Umwelt / Energy & Environment

Band / Volume 515

---

ISSN 1866-1793

ISBN 978-3-95806-507-9

# Contents

<b>Kurzfassung</b>	<b>iii</b>
<b>Abstract</b>	<b>v</b>
<b>Nomenclature</b>	<b>vi</b>
<b>Contents</b>	<b>viii</b>
<b>1 Introduction</b>	<b>1</b>
<b>2 Theory</b>	<b>5</b>
2.1 Nuclear fusion reactors . . . . .	5
2.2 Tungsten for fusion reactors . . . . .	7
2.3 Tungsten fiber-reinforced tungsten ( $W_f/W$ ) . . . . .	8
2.4 Chemical vapor deposition (CVD) . . . . .	10
2.5 Tungsten CVD reaction kinetics . . . . .	11
<b>3 Modeling and validation of W-CVD on single fibers</b>	<b>15</b>
3.1 Experimental . . . . .	15
3.1.1 Setup . . . . .	15
3.1.2 Procedure . . . . .	16
3.1.3 Evaluation . . . . .	19
3.2 Model . . . . .	22
3.2.1 COMSOL Multiphysics . . . . .	22
3.2.2 Model geometry . . . . .	23
3.2.3 Fluid dynamics . . . . .	23
3.2.4 Diffusion . . . . .	24
3.2.5 Heat transfer . . . . .	26
3.2.6 Chemistry and rate equations . . . . .	26
3.3 Experimental vs. simulated results . . . . .	28
3.4 Discussion . . . . .	34
3.5 Simulation enhanced input for the Arrhenius plot . . . . .	37
3.6 Chapter summary and conclusions . . . . .	40

<b>4</b>	<b>Modeling and validation of W-CVD between multiple fibers</b>	<b>41</b>
4.1	Experimental . . . . .	42
4.1.1	Substrate production (fabric weaving) . . . . .	42
4.1.2	Setup and procedure . . . . .	42
4.1.3	Sample selection and evaluation . . . . .	44
4.2	Reactor Model . . . . .	48
4.2.1	Model description . . . . .	48
4.2.2	Results . . . . .	51
4.3	Single Pore Model . . . . .	56
4.3.1	Model description . . . . .	56
4.3.2	Results . . . . .	66
4.4	Experimental vs. simulated results . . . . .	66
<b>5</b>	<b>Parameter studies towards relative density and fiber volume fraction</b>	<b>71</b>
5.1	Physical CVD parameter variation . . . . .	71
5.2	Fabric geometry parameter variation . . . . .	75
<b>6</b>	<b>Grain morphology of the CVD-W</b>	<b>79</b>
6.1	Influence of the grain size on the mechanical properties . . . . .	79
6.2	Literature review: influence of the CVD parameters on the grain size . . . . .	80
6.3	Experimental procedure . . . . .	81
6.3.1	Sample evaluation . . . . .	81
6.4	Grain width results . . . . .	84
6.4.1	H <sub>2</sub> partial pressure variation . . . . .	84
6.4.2	WF <sub>6</sub> partial pressure variation . . . . .	85
6.4.3	Temperature variation . . . . .	85
6.4.4	Overview plot: grain width vs. varied parameters . . . . .	86
6.5	Chapter conclusions . . . . .	88
<b>7</b>	<b>Using the gained knowledge to improve W<sub>f</sub>/W</b>	<b>89</b>
7.1	Deciding the fabric geometry parameters . . . . .	89
7.2	Deciding the CVD process parameters . . . . .	90
7.3	Experimental W <sub>f</sub> /W results applying the new parameters . . . . .	93
<b>8</b>	<b>Thesis conclusions and outlook</b>	<b>95</b>
<b>9</b>	<b>Appendix</b>	<b>I</b>
9.1	Material and species properties . . . . .	I
9.2	Detailed results for the single fiber setup . . . . .	II

*Contents*

9.3	Microscopic image analysis of $W_f/W$ . . . . .	III
9.3.1	Masking procedure . . . . .	III
9.3.2	Python script and detailed results . . . . .	IV
9.4	Python script for the thermal diffusion coefficient . . . . .	X
9.5	Python script for theoretical $\Phi_{V_f}$ and $\rho_{rel}$ as function of fiber positions (uniform growth) . . . . .	XIII
<b>List of Figures</b>		<b>XVII</b>
<b>List of Tables</b>		<b>XXIII</b>
<b>Bibliography</b>		<b>XXV</b>
<b>Acknowledgments</b>		<b>XXXVII</b>

Energie & Umwelt / Energy & Environment  
Band / Volume 515  
ISBN978-3-95806-507-9

Mitglied der Helmholtz-Gemeinschaft

