**Supplementary material for**:

F. Riedlsperger, B. Gsellmann, E. Povoden-Karadeniz, O. Tassa, S. Matera, M. Domankova, F. Kauffmann, E. Kozeschnik and B. Sonderegger, “*Thermodynamic modelling and microstructural study of Z-phase formation in a Ta-alloy martensitic steel* ”, MDPI Materials 2021, 14, xx

*Part 1 (this document):* Thermodynamic parameters and diffusion mobilities to be included in open source steel databases“mc\_fe.tdb” and “mc\_fe.ddb”, see online: <https://www.matcalc.at/index.php/databases/open-databases>

*Part 2 (Excel file):* MatCalc simulation data (equilibrium results of ZULC and Z6 as well as precipitate kinetic results of Z6)

**Part 1:**

1. Thermodynamic parameters:

$ Definition of element   
ELEMENT TA BCC\_A2 80.9479 5681.872 41.4718 !

$ MatCalc specific commands  
ADD\_COMPOSITION\_SET FCC\_A1 :TA,TI,NB,V:C,N: !  
ADD\_COMPOSITION\_SET HCP\_A3 :CR,TA:N: !  
ADD\_COMPOSITION\_SET HCP\_A3 :MO:C: !  
ADD\_COMPOSITION\_SET HCP\_A3 :CR,V:C: !

$ Phase descriptions  
PHASE BCC\_A2 %& 2 1 3 !  
 CONSTITUENT BCC\_A2 : CO,CR,CU,FE%,MN,MO,NI,SI,TA,V,W :B,C,N,VA% : !  
 PARAMETER G(BCC\_A2,TA:N;0) 273.00 +500000+GHSERTA#+3\*GHSERNN#; 6000.00 N  
 PARAMETER L(BCC\_A2,TA:N,VA;1) 273.00 +1250000-280\*T; 6000.00 N

PHASE FCC\_A1 %' 2 1 1 !  
 CONSTITUENT FCC\_A1 : CO,CR,CU,FE%,MN,MO,NI,SI,TA,V,W :B,C,N,VA% : !  
 PARAMETER G(FCC\_A1,TA:C;0) 273.00 +GHSERTA#+GHSERCC#-50000-60\*T; 6000.00 N  
 PARAMETER G(FCC\_A1,TA:N;0) 273.00 +GHSERTA#+GHSERNN#-190000+95\*T; 6000.00 N  
 PARAMETER L(FCC\_A1,TA:N,VA;0) 273.00 +1e-8; 6000.00 N  
 PARAMETER L(FCC\_A1,CR,TA:N;0) 273.00 -55000; 6000.00 N

PHASE HCP\_A3 %) 2 1 0.5 !  
 CONSTITUENT HCP\_A3 : CO,CR,CU,FE%,MN,MO,NI,SI,TA,V,W :B,C,N,VA% : !  
 PARAMETER G(HCP\_A3,TA:C;0) 273.00 +GHSERTA#+0.5\*GHSERCC#-100000+15\*T;   
6000.00 N  
 PARAMETER L(HCP\_A3,CR,TA:VA;0) 273.00 -25000; 6000.00 N  
 PARAMETER G(HCP\_A3,TA:N;0) 273.00 +1\*GHSERTA#+0.5\*GHSERNN#-75000+30\*T;   
6000.00 N  
PARAMETER L(HCP\_A3,CR,TA:N;0) 273.00 -25000; 6000.00 N  
PARAMETER L(HCP\_A3,TA:N,VA;0) 273.00 -25000; 6000.00 N

PHASE ZET % 3 1 1 1 !   
 CONSTITUENT ZET : CR%,FE : CR,NB,MO,TA,V : N%,VA : !  
 PARAMETER G(ZET,CR:CR:N;0) 273.00 +GHSERCR#+GHSERCR#+GHSERNN#+15000; 6000.00 N  
 PARAMETER G(ZET,CR:CR:VA;0) 273.00 +GHSERCR#+GHSERCR#+20000; 6000.00 N  
 PARAMETER G(ZET,CR:TA:N;0) 273.00 -25000+102\*T+GHSERCR#+GHSERTA#+GHSERNN#; 6000.00 N  
 PARAMETER G(ZET,CR:TA:VA;0) 273.00 +GHSERCR#+GHSERTA#; 6000.00 N  
 PARAMETER L(ZET,CR:TA:N,VA;0) 273.00 -200000+85\*T; 6000.00 N  
 PARAMETER G(ZET,CR:CR,TA:N;0) 273.00 -110000+18\*T; 6000.00 N

1. Diffusion mobilities:

PARAMETER MQ(FCC\_A1&TA,\*) 273.00 -QFE\_FCC+R\*T\*LN(5.0\*D0FE\_FCC); 6000.00 N !  
PARAMETER MQ(BCC\_A2&TA,\*) 273.00 -QFE\_BCC; 6000.00 N  
PARAMETER MF(BCC\_A2&TA,\*) 273.00 +R\*T\*LN(3.0\*D0FE\_BCC); 6000.00 N