ρ-CP: OPEN SOURCE DISLOCATION DENSITY BASED CRYSTAL PLASTICITY FRAMEWORK FOR SIMULATING TEMPERATURE- AND STRAIN RATE-DEPENDENT DEFORMATION

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This document provides a reference for the material properties/parameters used in the crystal plasticity model. Please refer to [1] for details of the constitutive model. The values for magnesium are given in `Mg_props.in`, those for copper are given in `fcc_props.in`, while those for tantalum are given in `bcc_props.in` in the respective simulation folders. Please refer to the line number corresponding to the material property/parameter. Note that in `DDCPStressUpdate.C` and `DDCPHCPStressUpdate.C`, the units of stress are in MPa, while those for dislocation density are in mm^{-2}. Please convert the units appropriately, while using them in the crystal plasticity model.

If the user desires to modify/add new parameters, this can be doing in `DDCPStressUpdate::assignProperties()` and `DDCPHCPStressUpdate::assignProperties()`.

Table 1: Anisotropic elastic constants for hcp magnesium [2], fcc OFHC copper [3, 4] and bcc tantalum [5]. Note that temperature effects on the elastic constants are only considered for tantalum, while the room temperature values are presented for magnesium and OFHC copper.

Parameter	Magnesium	line no. (`Mg_props.in`)	Copper	line no. (`fcc_props.in`)	Tantalum	line no. (`bcc_props.in`)
$C_{11}\,(GPa)$	59.4	1	170.0	1	268.2	1
$\frac{dC_{11}}{dT}\left(\frac{GPa}{K}\right)$	-	2	-	2	0.024	2
$C_{12}\,(GPa)$	25.6	3	124.0	3	159.6	3
$\frac{dC_{12}}{dT}\left(\frac{GPa}{K}\right)$	-	4	-	4	0.011	4
$C_{13}\,(GPa)$	21.4	5	-	-	-	-
$\frac{dC_{13}}{dT}\left(\frac{GPa}{K}\right)$	-	6	-	-	-	-
$C_{33}\,(GPa)$	61.6	7	-	-	-	-
$\frac{dC_{33}}{dT}\left(\frac{GPa}{K}\right)$	-	8	-	-	-	-
$C_{44}\,(GPa)$	16.4	9	75.0	6	87.1	5
$\frac{dC_{44}}{dT}\left(\frac{GPa}{K}\right)$	-	10	-	6	0.015	6
$G\,(GPa)$	16.4	11	41.5	7	87.1	7
$\frac{dG}{dT}\left(\frac{GPa}{K}\right)$	-	12	-	8	0.015	8

Table 2: Constitutive model parameters for magnesium (`Mg_props.in`).

Parameter	Basal	line no.	Prismatic	line no.	Pyramidal $\langle a \rangle$	line no.	Pyramidal $\langle c+a \rangle$	line no.	Tensile twin	line no.
$b^\alpha\,(nm)$	0.321	14	0.321	36	0.612	58	0.612	80	-	-
$\dot{\gamma}_{0s}^\alpha\,(s^{-1})$	1.0	15	1.0×10^{-2}	37	40	59	1.0×10^{-3}	81	-	-
ΔF^α	0.11 Gb^3	16	0.2 Gb^3	38	1.43 Gb^3	60	0.1 Gb^3	82	-	-
p^α	0.2	17	0.2	39	0.3	61	0.2	83	-	-
q^α	1.7	18	1.7	40	1.5	62	1.7	84	-	-
τ_{0s}^α (MPa)	2.0	19	21.0	41	50.0	63	38.0	85	-	-
s_t^α (MPa)	5.0	22	21.0	44	100.0	66	5.0	88	-	-
k_ρ^α	0.35	24	0.535	46	0.35	68	0.35	90	-	-
$A^{\alpha\alpha}$, $A^{\alpha\zeta}$	1.0, 0.2	26	1.0, 0.2	48	1.0, 0.2	70	1.0, 0.2	92	-	-
$\rho_m^0\,(m^{-2})$	1×10^{10}	27	1×10^{10}	49	1×10^{10}	71	1×10^{10}	93	-	-
$\rho_i^0\,(m^{-2})$	1×10^{10}	28	1×10^{10}	50	1×10^{10}	72	1×10^{10}	93	-	-
k_M^α	0.0017	30	1.0	52	1.0	74	3.5	96	-	-
$R_c^\alpha\,(nm)$	19.386	31	19.386	53	19.386	75	36.462	97	-	-
k_I^α	0.0015	25	0.98	47	0.8	69	3.4	91		
k_D^α	0.5	33	180	55	500	77	350	99	-	-
$\dot{\gamma}_{0t}^\alpha\,(s^{-1})$	-	-	-	-	-	-	-	-	1.0×10^{-3}	104
τ_{0t}^α (MPa)	-	-	-	-	-	-	-	-	2.0	102
D_0^α (MPa)	-	-	-	-	-	-	-	-	10.0	103
m^α	-	-	-	-	-	-	-	-	20	105
γ_{tw}^α	-	-	-	-	-	-	-	-	0.1289	106
h_0^α (MPa)	-	-	-	-	-	-	-	-	1000	108
m_{th}^α	-	-	-	-	-	-	-	-	10	109

Table 3: Constitutive model parameters for OFHC copper (`fcc_props.in`) and tantalum (`bcc_props.in`). Note that the tantalum model was not calibrated to any cyclic loading experiments and it was assumed that slip system-level backstress is not present.

Parameter	Copper	Tantalum	line no.
$b^\alpha\,(nm)$	0.256	0.286	9
$\dot{\gamma}_{0s}^\alpha\left(s^{-1}\right)$	4×10^6	1.73×10^7	10
ΔF^α	$0.25Gb^3$	$0.2Gb^3$	11
p^α	0.35	0.28	12
q^α	1.3	1.38	13
$\tau_{0s}^\alpha\,(\mathrm{MPa})$	0.0	24	14
$s_t^\alpha\,(\mathrm{MPa})$	38	386	17
k_ρ^α	0.2	0.3	19
$A^{\alpha\alpha}$, $A^{\alpha\zeta}$	1, 0.1	1, 0.1	21
$\rho_m^0\left(m^{-2}\right)$	5×10^{11}	1×10^{11}	22
$\rho_i^0\left(m^{-2}\right)$	5×10^{11}	1×10^{11}	23
k_M^α	0.13	0.05	25
$R_c^\alpha\,(nm)$	1.53	1.488	26
k_I^α	0.12	0.045	20
k_D^α	40	20	28
$k_{\chi1}^\alpha$	1100	-	29
$k_{\chi2}^\alpha$	1000	-	30

References

[1] Anirban Patra, Suketa Chaudhary, Namit Pai, Tarakram Ramgopal, Sarthak Khandelwal, Adwitiya Rao, and David L McDowell. ρ-cp: Open source dislocation density based crystal plasticity framework for simulating temperature-and strain rate-dependent deformation. *Computational Materials Science*, 224:112182, 2023.

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[4] PD Wu, KW Neale, and Erik Van der Giessen. Simulation of the behaviour of fcc polycrystals during reversed torsion. *International Journal of Plasticity*, 12(9):1199–1219, 1996.

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