

Experimental and simulation study of grain boundaries in UO₂: supplementary data

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CSL denomination (from GBStudio [22])	Geometrical characteristics			Empirical potential			
	Axis	Angle	Plane	Morelon	Yakub	Pota	Cooper
$\Sigma 3$ {111}/[111]	111	60°	111	0.94	1.04	0.83	1.08
$\Sigma 5$ {012}/[100]	100	36.86°	012	1.73	1.42	1.85	1.28
$\Sigma 7$ {3-2-1}/[111]	111	38.21°	3-2-1	1.53	1.58	1.64	1.58
$\Sigma 9$ {2-2-1}/[110]	110	38.94°	2-2-1	1.57	1.58	1.55	1.56
$\Sigma 11$ {1-13}/[110]	110	50.47°	1-13	0.91	1.07	0.9	1.13
$\Sigma 13a$ {023}/[100]	100	22.62°	023	1.53	1.75	1.7	1.72
$\Sigma 13b$ {4-3-1}/[111]	111	27.79°	4-3-1	1.52	1.77	1.69	1.68
$\Sigma 15$ {1-25}/[210]	210	48.19°	1-25	1.57	1.79	1.65	1.79
$\Sigma 17a$ {041}/[100]	100	28.07°	041	1.69	1.89	1.84	1.7
$\Sigma 17b$ {3-2-2}/[221]	221	61.9°	3-2-2	1.68	1.95	1.75	1.93
$\Sigma 19a$ {3-3-1}/[110]	110	26.53°	3-3-1	1.37	1.52	1.42	1.51
$\Sigma 19b$ {5-3-2}/[111]	111	46.8°	5-3-2	1.63	1.82	1.79	1.8
$\Sigma 21a$ {5-4-1}/[111]	111	21.78°	5-4-1	1.43	1.64	1.49	1.62
$\Sigma 21b$ {1-42}/[211]	211	44.4°	1-42	-	-	-	1.68
$\Sigma 23$ {1-63}/[311]	311	40.45°	1-63	1.6	1.78	1.74	1.73
$\Sigma 25a$ {034}/[100]	100	16.26°	034	1.77	1.56	1.44	1.6
$\Sigma 25b$ {5-4-3}/[331]	331	51.7°	5-4-3	-	-	-	1.82
$\Sigma 27a$ {1-15}/[110]	110	31.59°	1-15	1.55	1.73	1.62	1.72
$\Sigma 27b$ {1-27}/[210]	210	35.43°	1-27	1.63	1.83	1.79	1.82
$\Sigma 29a$ {052}/[100]	100	43.6°	052	1.67	1.84	1.94	1.72
$\Sigma 31b$ {2-73}/[211]	211	52.2°	2-73	-	-	-	1.68
$\Sigma 33c$ {2-25}/[110]	110	59°	2-25	1.36	1.7	1.44	1.67
$\Sigma 39b$ {2-30}/[321]	321	50.1°	2-30	-	-	-	1.82
$\Sigma 41a$ {045}/[100]	100	12.68°	045	1.23	1.74	1.28	1.75
$\Sigma 41c$ {4-4-3}/[110]	110	55.9°	4-4-3	1.63	1.89	1.67	1.92
$\Sigma 45c$ {7-5-4}/[221]	221	53.1°	7-5-4	-	-	-	1.88

Figure 1. Geometrical characteristics of the CSL grain boundaries studied in this work and their formation energies (J.m⁻²).