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冲击载荷下 TATB 晶体滑移和各向异性的分子动力学研究

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The Slip and Anisotropy of TATB Crystal under Shock Loading *via* Molecular Dynamics Simulation

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表 S1　沿垂直于(101)、(111)、(011)、(110)、(010)和(100)晶面的冲击方向下潜在滑移系的 RSS 值

Table S1　The RSS values for the potential slip systems along shock directions normal to (101), (111), (011), (110), (010), and (100) planes

Shock plane	Slip system	RSS/GPa
(101)	{010}<100>	2.063
	{0-11}<100>	1.855
	{130}<3-13>	1.795
	{140}<4-14>	1.787
	{120}<2-12>	1.773
	{041}<100>	1.702
	{-210}<001>	1.678
	{-310}<001>	1.699
	{-410}<001>	1.642
	{001}<120>	0.330
	{001}<110>	0.219
	{001}<100>	0.143
(111)	{-310}<130>	4.362
	{-410}<140>	4.248
	{-140}<410>	4.129
	{-130}<310>	4.095
	{-210}<120>	4.093
	{110}<001>	3.624
	{-120}<210>	3.596
	{210}<001>	3.595
	{120}<001>	3.557
	{310}<001>	3.544
	{001}<010>	0.472
	{001}<120>	0.387
	{001}<110>	0.190
(011)	{-110}<110>	2.739
	{410}<-144>	2.581
	{310}<-133>	2.565
	{210}<-122>	2.477
	{100}<011>	2.402
	{-110}<111>	2.347
	{401}<-144>	2.342
	{301}<-133>	2.258
	{001}<110>	0.245
	{001}<120>	0.213
	{001}<010>	0.120
(110)	{-130}<310>	4.266
	{-140}<410>	4.134

	{-310}<130>	4.114
	{-410}<140>	4.113
	{-120}<210>	4.111
	{-301}<010>	3.843
	{-401}<010>	3.804
	{-201}<010>	3.803
	{001}<100>	0.948
	{001}<010>	0.617
	{001}<110>	0.361
	{001}<120>	0.174
(010)	{-401}<010>	3.63
	{-301}<010>	3.623
	{100}<010>	3.398
	{410}<-140>	3.293
	{-120}<210>	3.211
	{310}<-130>	3.178
	{210}<-120>	2.904
	{-110}<110>	2.791
	{001}<010>	0.299
	{001}<1-20>	0.298
	{001}<1-10>	0.284
(100)	{-110}<110>	2.715
	{120}<-210>	2.572
	{130}<-310>	2.502
	{140}<-410>	2.420
	{010}<101>	2.130
	{041}<4-14>	2.030
	{0-41}<100>	1.990
	{0-31}<100>	1.988
	{031}<3-13>	1.957
	{0-21}<100>	1.914
	{001}<110>	0.381
	{001}<120>	0.375

S2 沿垂直于(101)、(111)、(011)、(110)、(010)和(100)晶面的冲击方向下潜在滑移系的 MD 模拟结果

Table S2 MD simulation results for the potential slip systems along the shock directions normal to (101), (111), (011), (110), (010), and (100) planes

Shock plane	Slip system	τ_0/GPa	$\tau_{barrier}$/GPa	T/K	$t_{reaction}$/ps	N_{TATB}/%
(101)	{010}<100>	2.310	12.035	1538	0.80	0.61
	{0-11}<100>	1.778	9.367	1320	0.80	1.95
	{130}<3-13>	1.832	7.204(2.387)	1504	1.30	0.26

	{140}<4-14>	1.810	6.812	1418	0.80	1.25
	{120}<2-12>	1.920	8.221	1580	1	0
	{041}<100>	1.802	8.303	1309	1.05	2.15
	{-210}<001>	1.713	5.379	1406	1.10	3.71
	{-310}<001>	1.698	3.987	1366	1.20	3.91
	{-410}<001>	1.678	3.913	1356	1.85	4.69
	{001}<120>	0.179	0.753(0.813/1.033)	459		100
	{001}<110>	0.154	0.454(0.908/1.015)	482		100
	{001}<100>	0.119	0.406(1.020)	470		100
	{-310}<130>	4.306	7.679	1657	0.50	0
	{-410}<140>	4.241	7.636	1612	0.55	0
	{-140}<410>	4.033	7.443	1577	0.55	0.43
	{-130}<310>	3.855	7.349	1583	0.60	0.17
	{-210}<120>	4.125	7.297	1709	0.45	0
	{110}<001>	3.861	3.759(4.195)	1278	0.55	14.39
(111)	{-120}<210>	3.209	6.799	1630	0.60	0
	{210}<001>	4.085	2.871(3.272)	1263	0.80	13.98
	{120}<001>	3.606	2.565(7.099)	1402	0.70	14.58
	{310}<001>	3.759	3.027(2.969)	1226	0.55	18.16
	{001}<010>	0.345	0.850	502		100
	{001}<120>	0.360	0.905	494	8	99.92
	{001}<110>	0.294	0.929(0.797)	532	8	99.94
	{-110}<110>	3.002	11.357	1617	0.70	0
	{410}<-144>	2.883	7.186	1414	1.20	0.35
	{310}<-133>	2.842	8.103	1521	0.80	0.26
	{210}<-122>	2.660	10.274	1617	0.85	0
	{100}<011>	2.780	5.237	1383	1.30	3.13
(011)	{-110}<111>	2.620	6.701	1331	1.85	6.08
	{401}<-144>	2.127	7.926	1470	1.35	2.17
	{301}<-133>	2.340	9.537	1527	1.60	0.78
	{001}<110>	0.216	2.017(1.052/1.171)	576	8	99.94
	{001}<120>	0.234	1.637(1.617/0.875)	540		100
	{001}<010>	0.134	0.681(0.538/0.712)	552		100
	{-130}<310>	4.002	8.001	1709	0.65	0
	{-140}<410>	3.985	8.002	1756	0.75	0
	{-310}<130>	4.050	5.925	1576	0.30	0
	{-410}<140>	3.906	6.986	1618	0.65	0
	{-120}<210>	4.054	7.296	1788	0.65	0
(110)	{-301}<010>	4.334	3.914	1498	0.55	0.21
	{-401}<010>	4.142	3.779	1480	0.65	0.50
	{-201}<010>	3.681	4.599	1466	0.60	0.49
	{001}<100>	0.835	0.423(0.769/0.775)	617	4.10	98.76
	{001}<010>	0.309	0.601(0.235/0.482)	565	7.20	98.73
	{001}<110>	0.398	1.797(0.899)	699	1.85	94.51

	{001}<120>	0.198	1.544(0.482)	615	2.30	95.19
(010)	{-401}<010>	3.205	4.226	1453	0.90	0.28
	{-301}<010>	3.712	5.135	1556	0.50	0
	{100}<010>	2.705	5.671	1465	0.95	0.35
	{410}<-140>	3.126	4.349	1466	0.80	0.28
	{-120}<210>	3.214	6.297	1662	0.65	0
	{310}<-130>	3.126	4.676	1506	0.80	0
	{210}<-120>	2.879	4.505	1471	0.80	0
	{-110}<110>	2.688	4.913	1449	0.70	0.26
	{001}<010>	0.310	1.565	673	2.25	95.70
	{001}<1-20>	0.329	1.704	623	6.00	98.96
	{001}<1-10>	0.356	1.424	598	7.60	99.65
(100)	{-110}<110>	2.935	4.274	1478	0.70	0
	{120}<-210>	2.601	3.794	1448	0.80	0.43
	{130}<-310>	2.496	5.013	1420	0.65	0
	{140}<-410>	2.665	4.690	1415	0.60	0.76
	{010}<101>	2.053	4.870	1231	1.60	21.98
	{041}<4-14>	2.008	4.388	1196	1.05	23.06
	0-41}<100>	2.373	4.525	1449	0.85	1.48
	{0-31}<100>	1.873	4.602	1391	0.80	0
	{031}<3-13>	2.016	3.989	1232	1.55	21.98
	{0-21}<100>	1.908	5.050	1410	1.25	0.78
	{001}<110>	0.384	2.366	684	4.6	96.39
	{001}<120>	0.307	1.733	655	6.75	99.17

$\tau_{barrier}$: shear stress barrier, τ_0 is the initial shear stress; T is measured at 4 ps; $t_{reaction}$: the time at which chemical reaction begins; N_{TATB} is measured at 8ps. The slip systems in bold are the ones that are likely to be activated.