Electronic Supplementary Information: Vacancy Induced Formation of Nanoporous Silicon, Carbon and Silicon Carbide

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This file contains tables with the statistical averages of configurations of nanoporous *a*-C, *a*-Si, *a*-SiC(3C), *a*-SiC(4H) and *a*-SiC(6H) at different densities, including the mean Third Peak Height (TPH) and Porosity Change (Porosity) between the initial and final configurations, along with the standard deviations ($\sigma_{\bar{x}}$). Also included are the bond length and angle distributions for all configurations, as a function of strain, for *a*-SiC(3C), *a*-SiC(4H) and *a*-SiC(6H). Bond type distributions for *a*-SiC(3C), *a*-SiC(4H) and *a*-SiC(6H), and bond length and angle distributions for *a*-C and *a*-Si are included in the main text. Conversion between density and strain can be calculated using the tables herein.

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Table S1: Statistical averages of configurations of nanoporous a-C at different densities, including the mean Third Peak Height (TPH) and Porosity change (Porosity), along with the standard deviations ($\sigma_{\bar{x}}$).

ρ (g/cm^3)	Strain (%)	Atoms	Vacancies	TPH (Arb.)	$\sigma_{\bar{TPH}}$	Porosity (Arb.)	$\sigma_{\bar{Porosity}}$
3.500	0.625	994	6	6.594	0.019	0.018	0.001
3.400	3.464	965	35	5.459	0.059	0.043	0.002
3.300	6.303	937	63	4.719	0.093	0.059	0.005
3.200	9.143	909	91	4.125	0.103	0.070	0.006
3.100	11.982	880	120	3.686	0.099	0.073	0.008
3.000	14.821	852	148	3.305	0.101	0.075	0.007
2.900	17.660	823	177	2.901	0.150	0.077	0.011
2.800	20.500	795	205	2.181	0.315	0.096	0.011
2.700	23.339	767	233	1.339	0.650	0.119	0.025
2.600	26.178	738	262	0.870	0.016	0.128	0.005
2.500	29.018	710	290	0.850	0.039	0.116	0.005

Table S2: Statistical averages of configurations of nanoporous a-Si at different densities, including the mean Third Peak Height (TPH) and Porosity change (Porosity), along with the standard deviations ($\sigma_{\bar{x}}$).

ρ (g/cm^3)	Strain (%)	Atoms	Vacancies	TPH (Arb.)	$\sigma_{\bar{TPH}}$	Porosity (Arb.)	$\sigma_{\bar{Porosity}}$
2.300	1.245	988	12	4.062	0.126	-0.001	0.003
2.270	2.533	975	25	3.702	0.179	0.001	0.003
2.240	3.821	962	38	3.432	0.063	0.007	0.005
2.210	5.109	949	51	3.232	0.180	0.007	0.009
2.200	5.539	945	55	3.035	0.179	0.017	0.015
2.190	5.968	940	60	2.882	0.305	0.026	0.022
2.180	6.398	936	64	2.251	0.734	0.076	0.061
2.170	6.827	932	68	2.229	0.664	0.076	0.054
2.160	7.256	927	73	1.643	0.676	0.121	0.061
2.150	7.686	923	77	0.970	0.182	0.175	0.023
2.140	8.115	919	81	0.889	0.097	0.182	0.017
2.130	8.544	915	85	0.845	0.025	0.177	0.009
2.100	9.833	902	98	0.833	0.022	0.168	0.006
2.070	11.121	889	111	0.853	0.019	0.143	0.012

Table S3: Statistical averages of configurations of nanoporous a-SiC(3C) at different densities, including the mean Third Peak Height (TPH) and Porosity change (Porosity), along with the standard deviations ($\sigma_{\bar{x}}$).

ρ (g/cm^3)	Strain (%)	Atoms	Vacancies	TPH (Arb.)	$\sigma_{\bar{TPH}}$	Porosity (Arb.)	$\sigma_{\bar{Porosity}}$
3.200	0.467	995	5	5.540	0.025	0.006	0.000
3.100	3.577	964	36	4.454	0.062	0.042	0.004
3.000	6.687	933	67	3.688	0.100	0.069	0.004
2.900	9.798	902	98	2.920	0.082	0.090	0.008
2.800	12.908	871	129	2.260	0.165	0.098	0.010
2.700	16.019	840	160	1.630	0.059	0.099	0.011
2.600	19.129	809	191	1.200	0.065	0.102	0.013
2.500	22.240	778	222	1.089	0.030	0.119	0.009
2.400	25.350	747	253	1.040	0.036	0.132	0.007
2.300	28.460	715	285	1.017	0.038	0.139	0.009
2.200	31.571	684	316	0.989	0.040	0.149	0.010
2.100	34.681	653	347	0.951	0.028	0.147	0.011
2.000	37.792	622	378	0.939	0.032	0.134	0.009
1.900	40.902	591	409	0.922	0.021	0.124	0.006
1.800	44.012	560	440	0.920	0.046	0.112	0.006
1.700	47.123	529	471	0.935	0.066	0.089	0.007

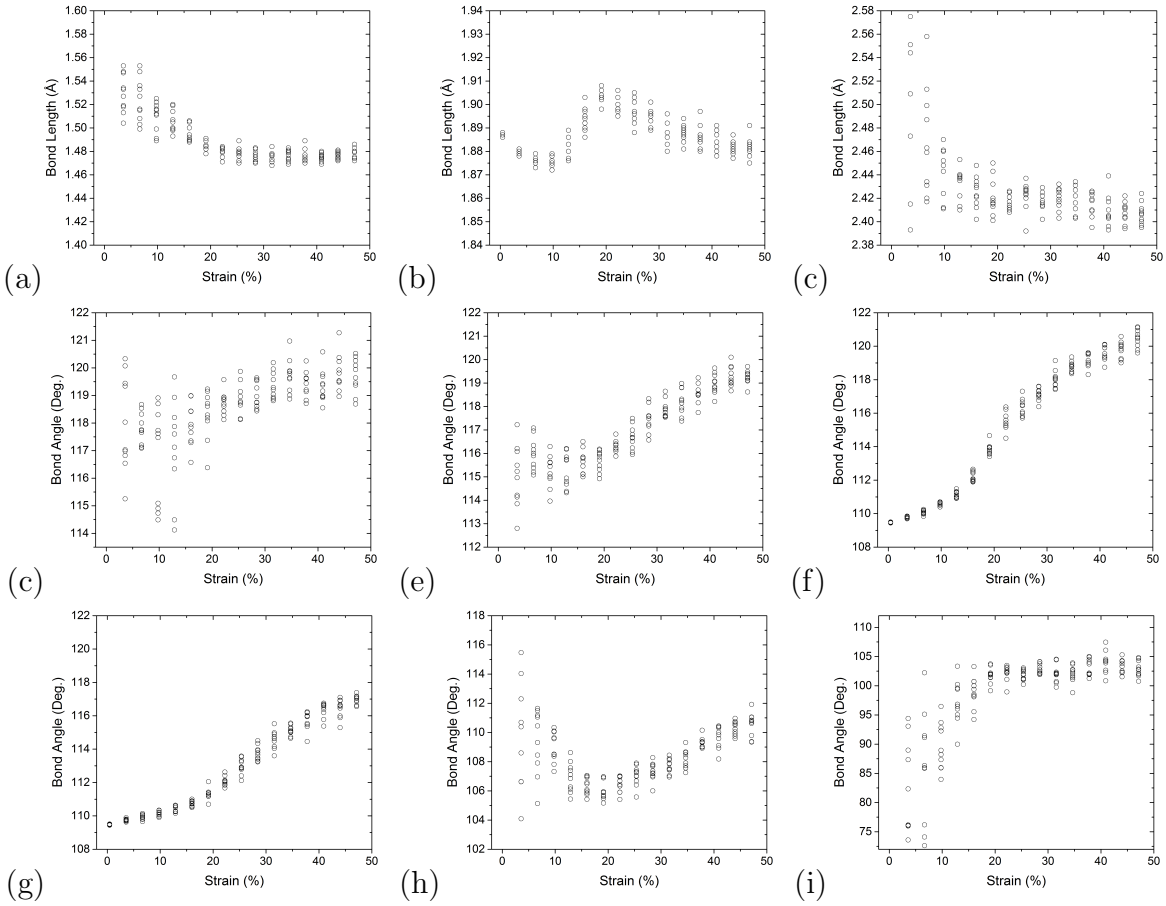

Figure S1: Local bonding environment of nanoporous *a*-SiC(3C), as a function of strain; including (a) the C–C bond length, (b) C–Si bond length, (c) Si–Si bond length, (d) C–C–C bond angle, (e) C–C–Si bond angle, (f) C–Si–C bond angle, (g) Si–C–Si bond angle, (h) C–Si–Si bond angle, and (i) Si–Si–Si bond angle.

Table S4: Statistical averages of configurations of nanoporous a-SiC(4H) at different densities, including the mean Third Peak Height (TPH) and Porosity change (Porosity), along with the standard deviations ($\sigma_{\bar{x}}$).

ρ (g/cm^3)	Strain (%)	Atoms	Vacancies	TPH (Arb.)	$\sigma_{\bar{TPH}}$	Porosity (Arb.)	$\sigma_{\bar{Porosity}}$
3.200	0.405	1020	4	4.850	0.018	0.008	0.001
3.100	3.517	988	36	3.940	0.041	0.050	0.003
3.000	6.629	956	68	3.239	0.077	0.078	0.004
2.900	9.742	924	100	2.640	0.088	0.102	0.004
2.800	12.854	892	132	1.970	0.094	0.109	0.009
2.700	15.966	861	163	1.430	0.082	0.113	0.013
2.600	19.079	829	195	1.162	0.057	0.109	0.011
2.500	22.191	797	227	1.080	0.022	0.123	0.009
2.400	25.303	765	259	1.050	0.027	0.133	0.011
2.300	28.416	733	291	1.010	0.036	0.142	0.010
2.200	31.528	701	323	1.000	0.021	0.152	0.005
2.100	34.641	669	355	0.970	0.032	0.147	0.008
2.000	37.753	637	387	0.930	0.033	0.135	0.011
1.900	40.865	606	418	0.934	0.029	0.121	0.008
1.800	43.978	574	450	0.906	0.035	0.109	0.006
1.700	47.090	542	482	0.935	0.039	0.094	0.005

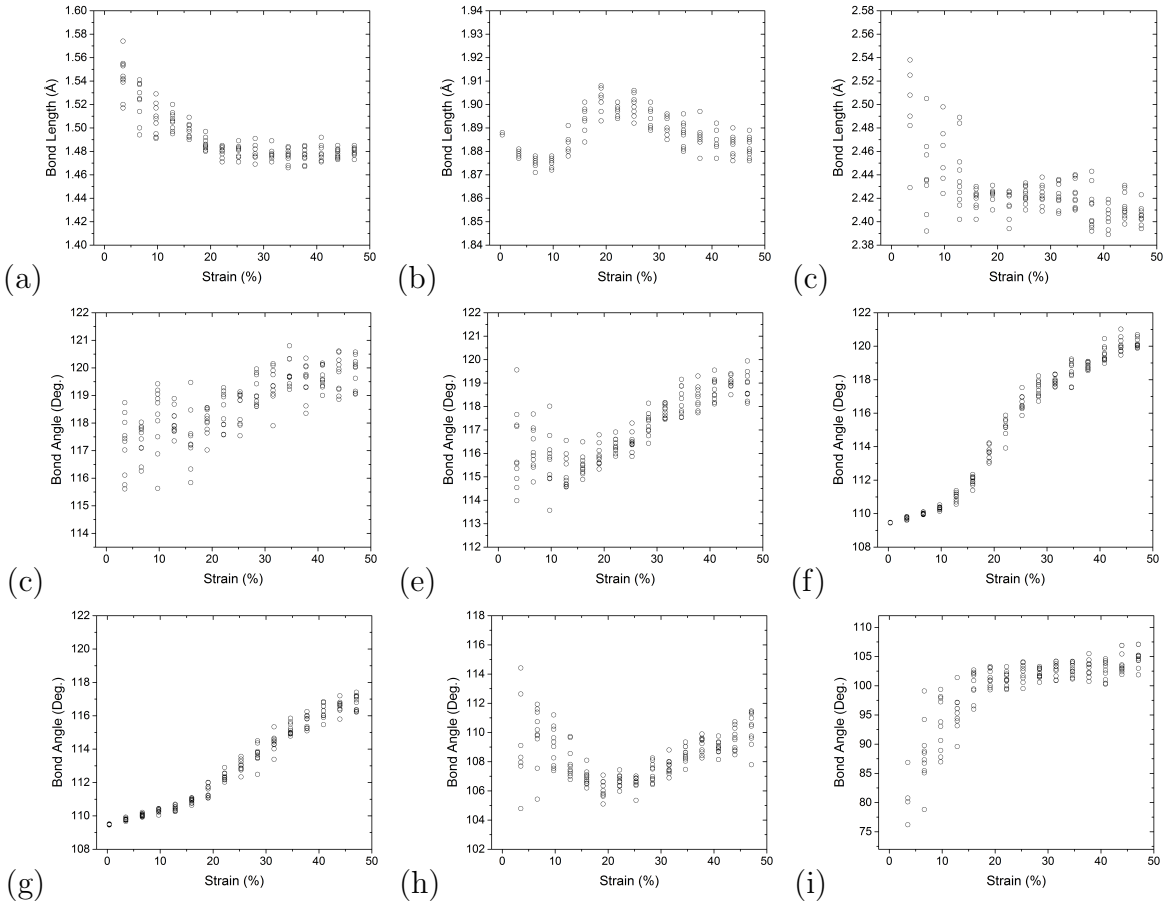

Figure S2: Local bonding environment of nanoporous *a*-SiC(4H), as a function of strain; including (a) the C–C bond length, (b) C–Si bond length, (c) Si–Si bond length, (d) C–C–C bond angle, (e) C–C–Si bond angle, (f) C–Si–C bond angle, (g) Si–C–Si bond angle, (h) C–Si–Si bond angle, and (i) Si–Si–Si bond angle.

Table S5: Statistical averages of configurations of nanoporous a-SiC(6H) at different densities, including the mean Third Peak Height (TPH) and Porosity change (Porosity), along with the standard deviations ($\sigma_{\bar{x}}$).

ρ (g/cm^3)	Strain (%)	Atoms	Vacancies	TPH (Arb.)	$\sigma_{\bar{TPH}}$	Porosity (Arb.)	$\sigma_{\bar{Porosity}}$
3.200	0.436	1147	5	5.095	0.016	0.006	0.001
3.100	3.547	1111	41	4.153	0.046	0.041	0.003
3.000	6.658	1075	77	3.366	0.076	0.064	0.004
2.900	9.770	1040	112	2.721	0.064	0.083	0.008
2.800	12.881	1004	148	2.143	0.109	0.093	0.009
2.700	15.993	968	184	1.501	0.070	0.089	0.007
2.600	19.104	932	220	1.184	0.067	0.094	0.007
2.500	22.215	896	256	1.063	0.020	0.102	0.009
2.400	25.327	860	292	1.019	0.023	0.117	0.012
2.300	28.438	824	328	1.019	0.023	0.132	0.005
2.200	31.549	789	363	0.960	0.025	0.134	0.007
2.100	34.661	753	399	0.947	0.033	0.135	0.005
2.000	37.772	717	435	0.933	0.027	0.124	0.005
1.900	40.884	681	471	0.925	0.047	0.117	0.008
1.800	43.995	645	507	0.933	0.029	0.099	0.006
1.700	47.106	609	543	0.926	0.024	0.088	0.006

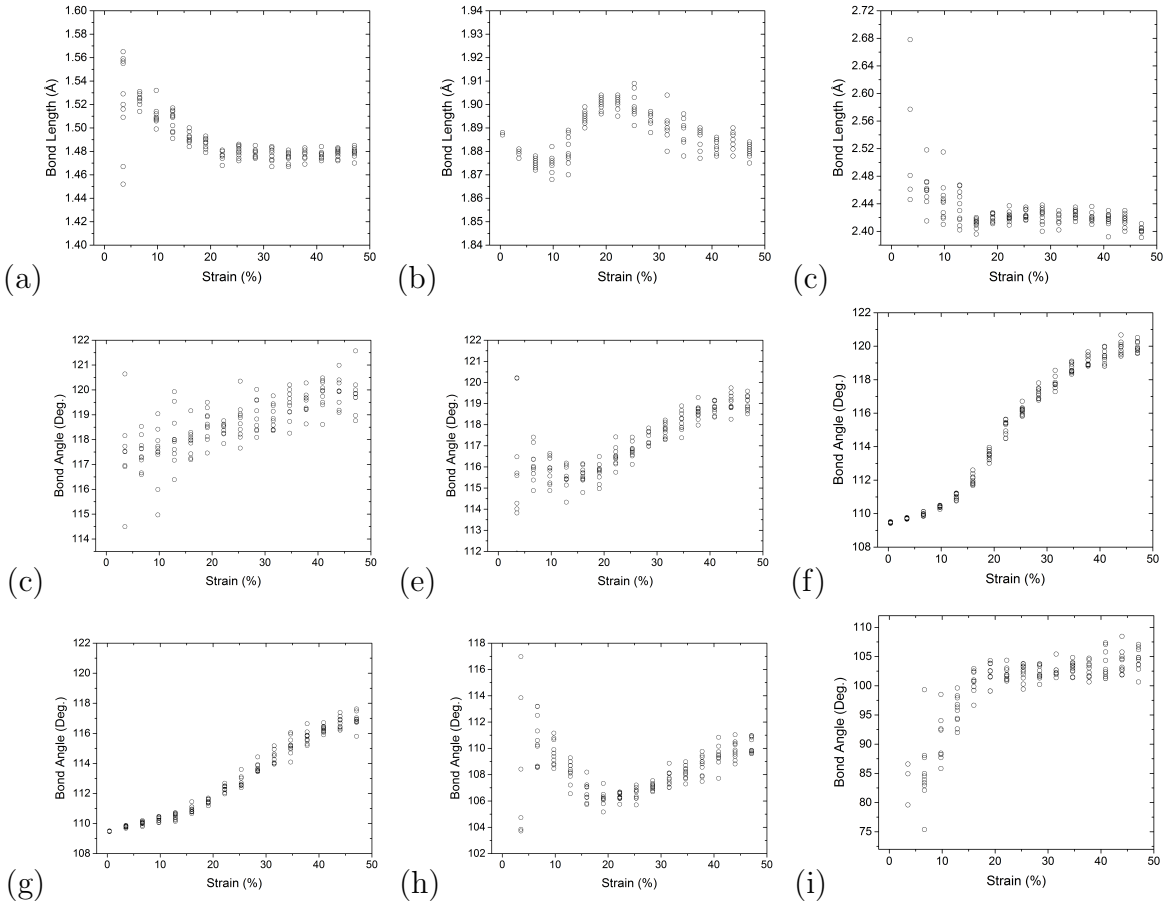

Figure S3: Local bonding environment of nanoporous *a*-SiC(6H), as a function of strain; including (a) the C–C bond length, (b) C–Si bond length, (c) Si–Si bond length, (d) C–C–C bond angle, (e) C–C–Si bond angle, (f) C–Si–C bond angle, (g) Si–C–Si bond angle, (h) C–Si–Si bond angle, and (i) Si–Si–Si bond angle.