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Strain Engineering of Polar Optical Phonon Scattering Mechanism – An Effective Way to Optimize the Power-factor and Lattice Thermal Conductivity of ScN

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Table S1. Mechanical, vibrational, and thermal properties obtained in ScN for different values of physical strain

		Strain % in SCN										
		+5	+4	+3	+2	+1	0	-1	-2	-3	-4	-5
Bulk modulus (GPa)	Voigt	158.903	175.364	193.885	214.289	236.318	260.501	286.578	314.958	346.020	379.743	416.343
	Reuss	158.903	175.364	193.885	214.289	236.318	260.501	286.578	314.958	346.020	379.743	416.343
	Average	158.903	175.364	193.885	214.289	236.318	260.501	286.578	314.958	346.020	379.743	416.343
Shear modulus (GPa)	Voigt	137.799	143.091	148.612	153.960	159.465	164.807	170.181	175.460	180.502	185.211	189.577
	Reuss	132.481	140.435	147.819	153.944	158.986	162.380	164.015	163.353	159.964	153.204	142.551
	Average	135.140	141.763	148.215	153.952	159.226	163.593	167.098	169.407	170.233	169.207	166.064
Young's modulus (GPa)	Voigt	320.696	337.483	355.106	372.638	390.549	408.313	426.182	443.942	461.294	477.932	493.785
	Reuss	311.010	332.538	353.595	372.607	389.591	403.335	413.213	417.825	415.815	405.130	383.845
	Average	315.853	335.010	354.351	372.622	390.070	405.824	419.698	430.883	438.555	441.531	438.815
Poisson ratio	Voigt	0.164	0.179	0.195	0.210	0.225	0.239	0.252	0.265	0.278	0.290	0.302
	Reuss	0.174	0.184	0.196	0.210	0.225	0.242	0.260	0.279	0.300	0.322	0.346
	Average	0.169	0.182	0.195	0.210	0.225	0.240	0.256	0.272	0.289	0.306	0.324
Transverse velocity (m/s)		6035.26703	6093.30263	6140.76965	6167.57162	6180.29813	6171.68019	6144.10942	6092.91532	6014.50809	5903.87665	5757.63389
Longitudinal velocity (m/s)		9560.08348	9768.97339	9980.33857	10181.63350	10373.88660	10556.46598	10727.34363	10886.58743	11034.54973	11166.87899	11283.28227
Average velocity (m/s)		6641.10062	6713.84858	6775.96685	6816.40468	6841.59864	6844.06791	6825.86398	6782.01404	6708.51548	6599.55135	6451.03938
Debye temperature (K)		836.72311	854.02229	870.29212	884.06907	896.12217	905.41006	912.12307	915.51110	914.92542	909.44027	898.33246
Minimum lattice thermal conductivity (W/mK) for Primitive cell n=2		2.40076	2.48412	2.56775	2.64843	2.72690	2.80187	2.87346	2.93932	2.99906	3.05036	3.09064
Minimum lattice thermal conductivity (W/mK) n=8		2.40078	2.48393	2.56773	2.64830	2.72712	2.80217	2.87351	2.93970	2.99947	3.05048	3.09116

Table S2. Indirect and direct band gaps obtained in ScN for different values of physical strain

Strain % in SCN	Indirect band gap (eV)	Direct band gap (eV)	E_{VBM} (eV)	E_{CBM} (eV)
+5	1.137	2.150	5.133	6.269
+4	1.115	2.137	5.349	6.464
+3	1.089	2.118	5.573	6.662
+2	1.060	2.094	5.805	6.864
+1	1.026	2.065	6.045	7.070
0	0.988	2.029	6.293	7.280
-1	0.945	1.986	6.549	7.494
-2	0.898	1.936	6.815	7.712
-3	0.845	1.878	7.090	7.935
-4	0.787	1.811	7.375	8.162
-5	0.723	1.735	7.670	8.393

Table S3. Material parameters used in the AMSET package

Strain	-2%	-1%	0%	+1%	+2%
Static dielectric constant $[\varepsilon_{sxx} = \varepsilon_{syy} = \varepsilon_{szz}]$	**17.6086**	**18.1724**	**18.8815**	**19.7622**	**20.8458**
High frequency dielectric constant $[\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz}]$	**7.8126**	**7.7236**	**7.6549**	**7.6054**	**7.5729**
Polar optical phonon effective frequency (THz)	**15.79**	**14.96**	**14.14**	**13.33**	**12.52**

*off- diagonal terms of the 3 x 3 dielectric tensors, ε_s and ε, are zero.

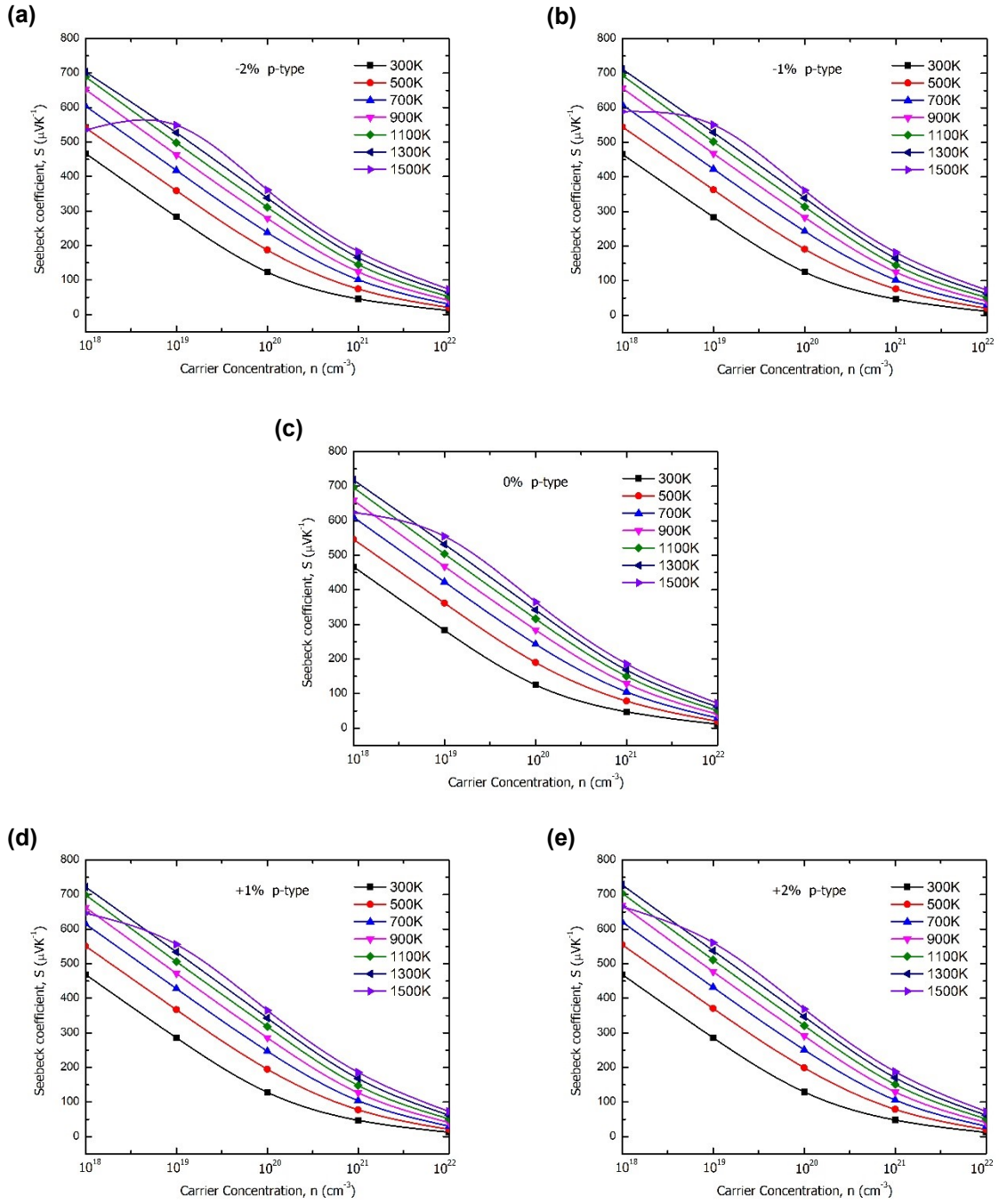

Figure S1. Seebeck coefficient versus carrier concentration in p-type ScN for different values of strains and temperatures

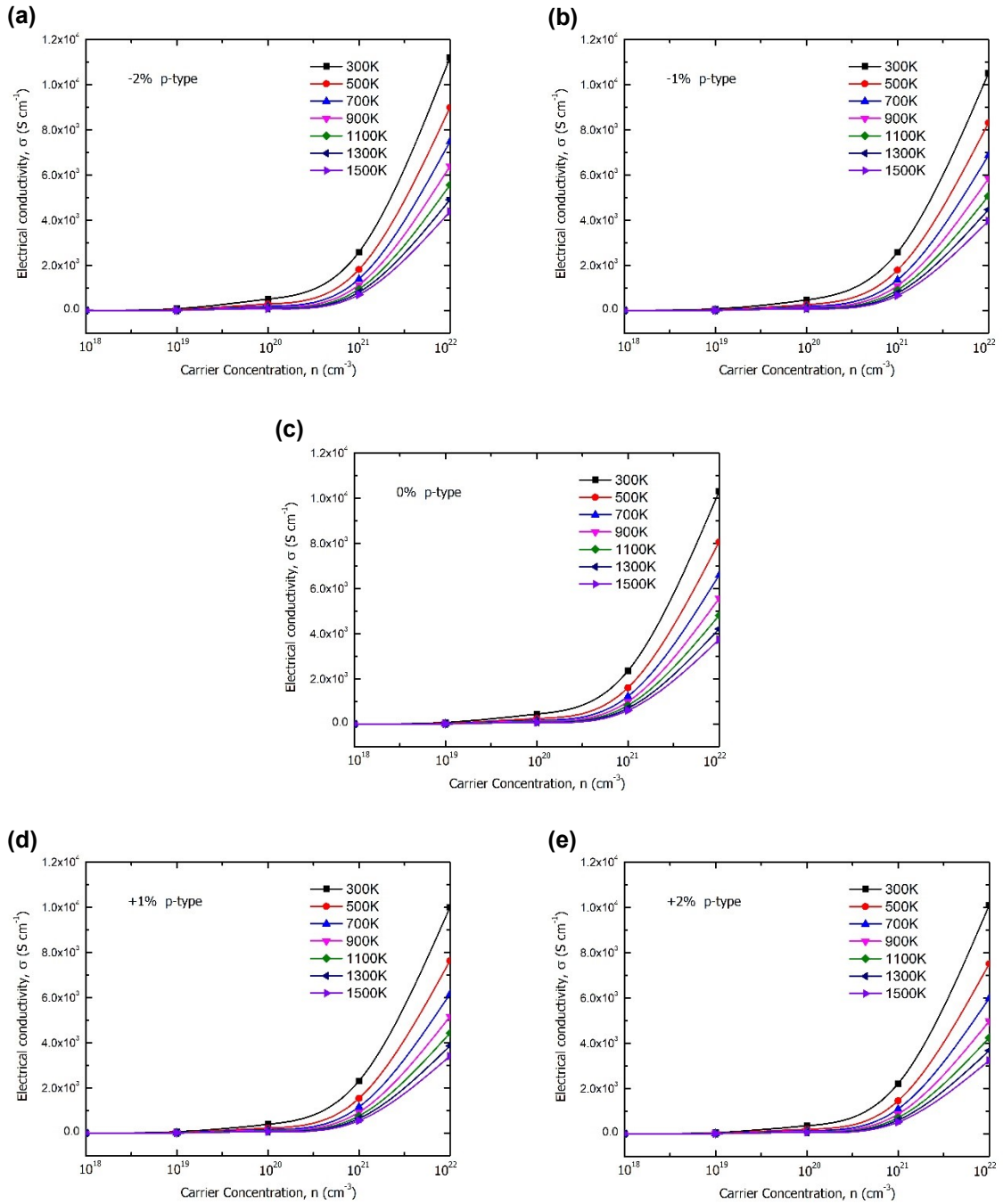

Figure S2. Electrical conductivity versus carrier concentration in p-type ScN for different values of strains and temperatures

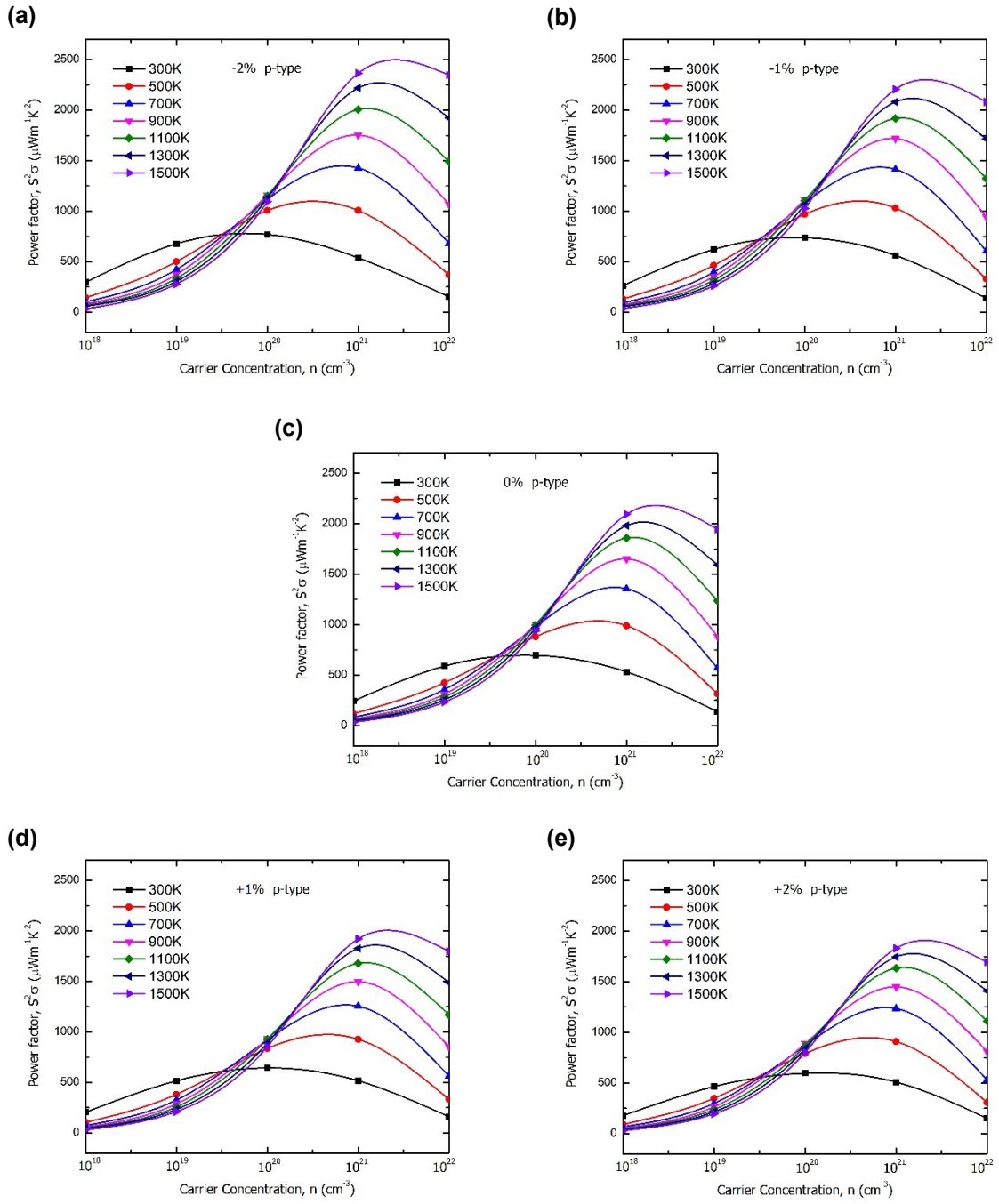

Figure S3. Power factor versus carrier concentration in p-type ScN for different values of strains and temperatures

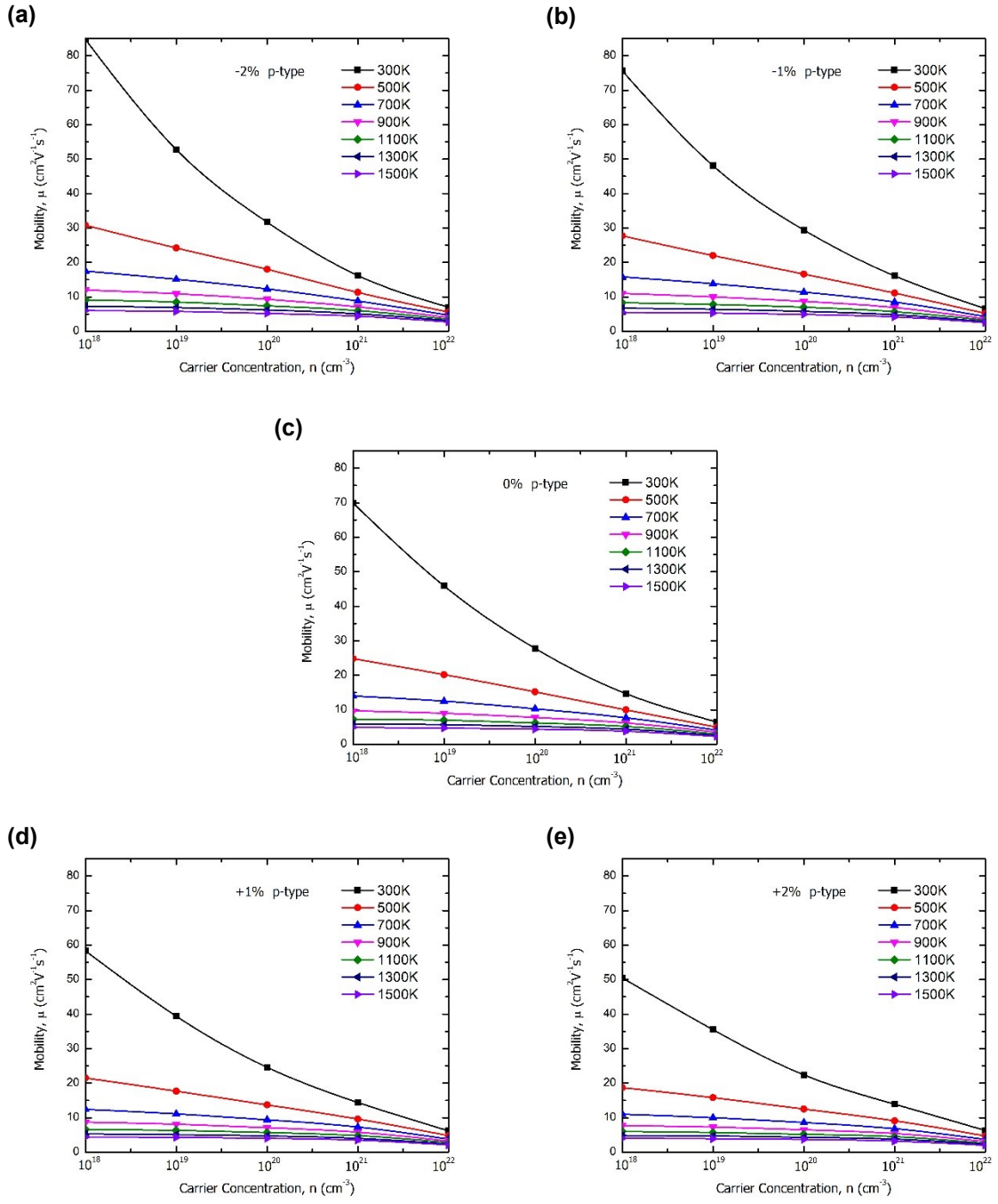

Figure S4. Mobility versus carrier concentration in p-type ScN for different values of strains and temperatures

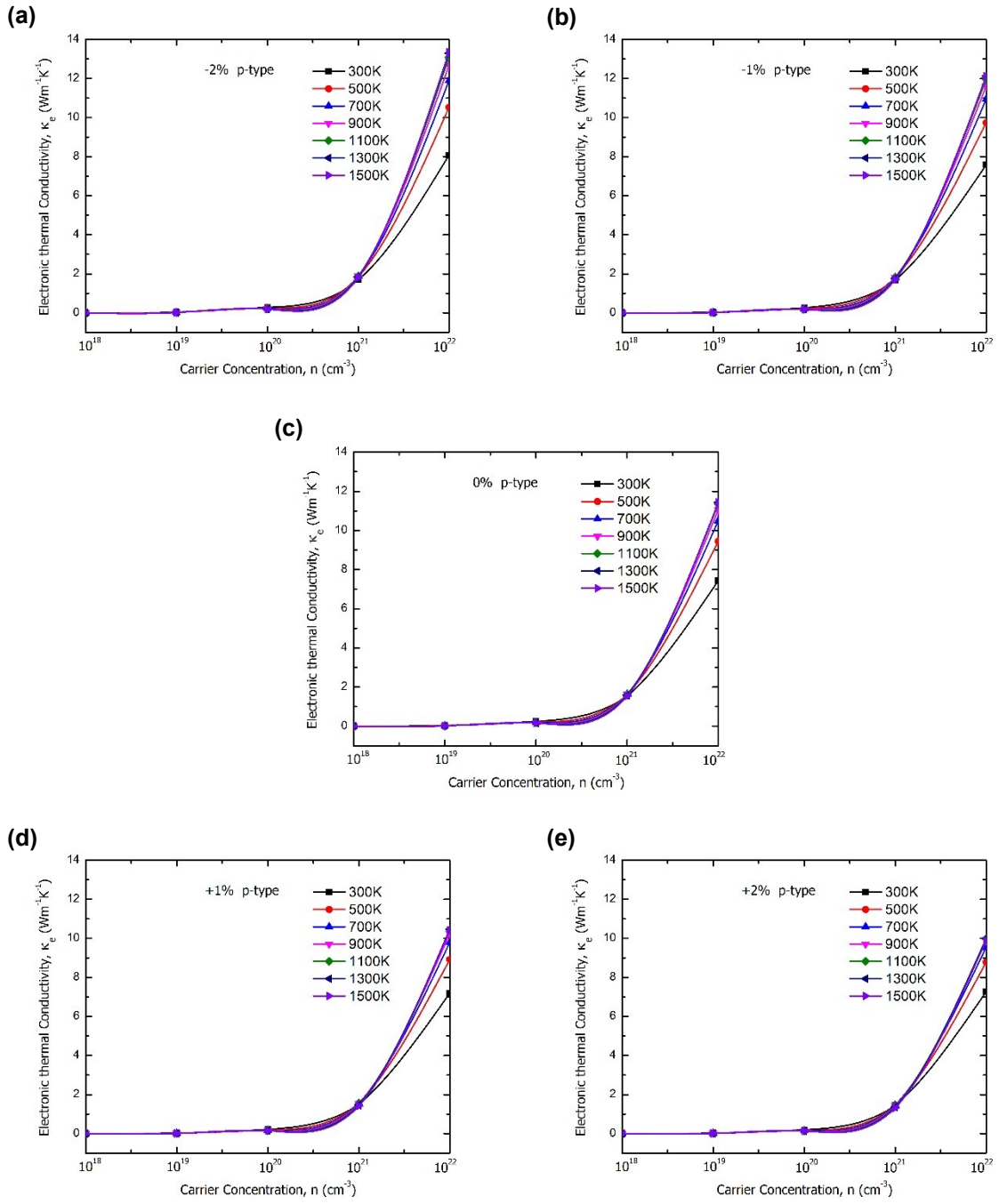

Figure S5. Electronic thermal conductivity versus carrier concentration in p-type ScN for different values of strains and temperatures

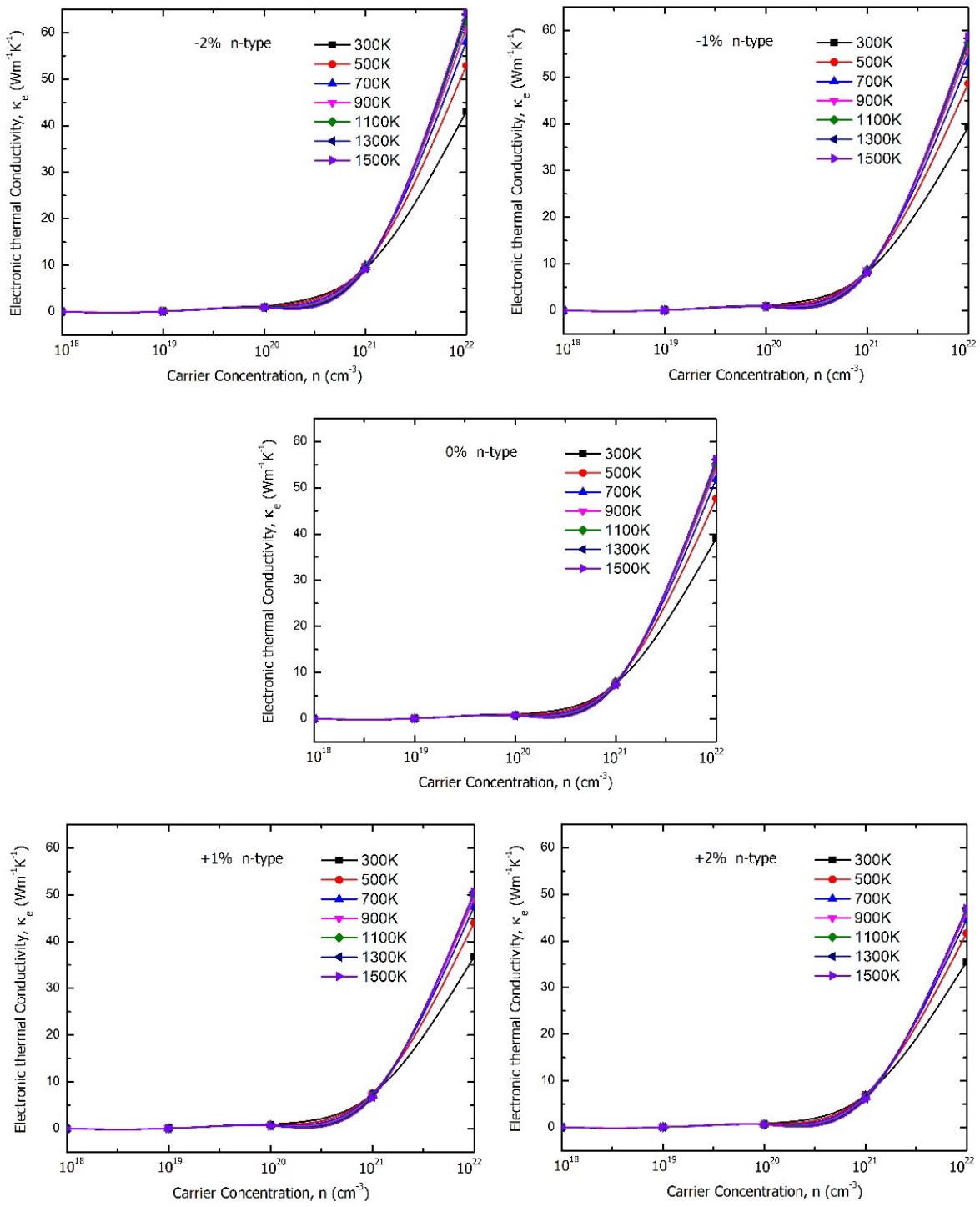

Figure S6. Electronic thermal conductivity versus carrier concentration in n-type ScN for different values of strains and temperatures