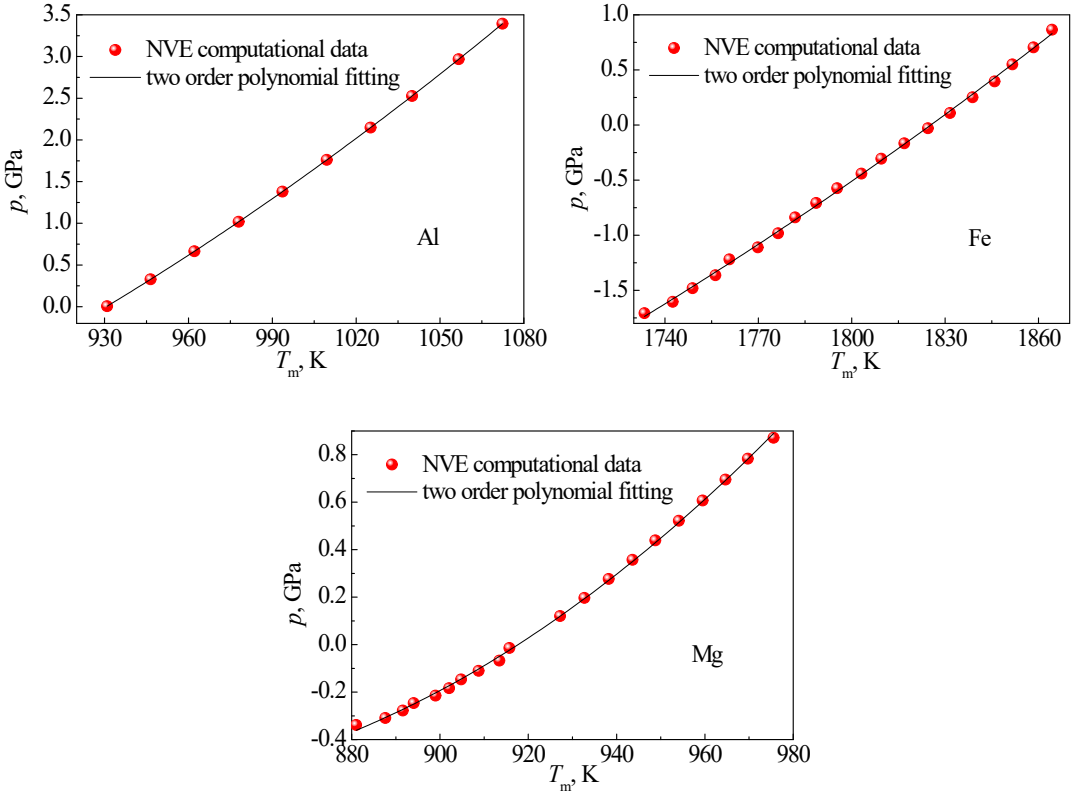
The calculations of NpH phase diagrams

Three steps are required to calculate the NpH phase diagram from the MD simulation.

1. Perform a series of NVE MD simulations (constant atomic number N, volume V and total energy E) of a solid-liquid bi-phase coexisting system to achieve the correlation of pressure and equilibrium melting point, p-T_m, and fit the computational experimental data with a second order polynomial. In this case, the pressure is achieved by adjusting the volume of the system.



2. From the fitted polynomials, we can computer a series of p_i-$T_{m,i}$ data pairs. Then, perform a series of NpT MD simulations (constant atomic number, pressure and temperature) of single crystal and liquid phases with the imposed p_i-$T_{m,i}$ conditions to achieve potential energy P_i, kinetic energy K_i and volume v_i, and finally the enthalpy H_i=P_i+K_i+p_iv_i.

Al

i	T	p	P_L	P_S	v_L	v_S	H_L	H_S
	K	GPa	eV/atom	eV/atom	Å^3/atom	Å^3/atom	eV/atom	eV/atom
1	930.89	0.005	-3.029	-3.141	18.701	17.728	-2.908	-3.020
2	946.46	0.328	-3.028	-3.139	18.594	17.657	-2.868	-2.980
3	962.12	0.665	-3.026	-3.137	18.491	17.583	-2.825	-2.940
4	977.99	1.018	-3.024	-3.134	18.383	17.507	-2.781	-2.896
5	993.65	1.380	-3.022	-3.131	18.278	17.430	-2.736	-2.852
6	1009.52	1.760	-3.019	-3.129	18.170	17.350	-2.689	-2.808
7	1025.18	2.148	-3.017	-3.126	18.063	17.269	-2.642	-2.762
8	1040	2.527	-3.014	-3.123	17.959	17.190	-2.596	-2.717
9	1056.71	2.967	-3.011	-3.119	17.843	17.101	-2.544	-2.665

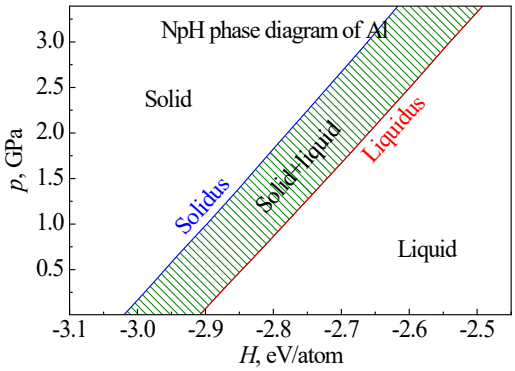
Fe

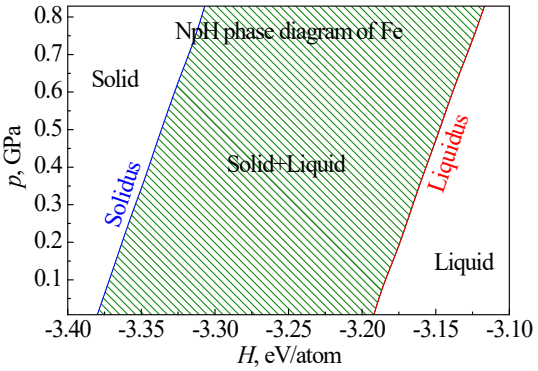
i	T K	p GPa	P_L eV/atom	P_S eV/atom	v_L Å^3/atom	v_S Å^3/atom	H_L eV/atom	H_S eV/atom
1	1825.67	0.007	-3.429	-3.617	13.162	12.290	-3.192	-3.380
2	1829.5	0.085	-3.429	-3.616	13.151	12.283	-3.186	-3.373
3	1833.95	0.178	-3.428	-3.616	13.140	12.276	-3.176	-3.365
4	1838.41	0.271	-3.428	-3.615	13.128	12.268	-3.168	-3.357
5	1842.86	0.365	-3.428	-3.614	13.114	12.261	-3.160	-3.348
6	1847.32	0.460	-3.427	-3.614	13.102	12.252	-3.151	-3.340
7	1851.51	0.550	-3.427	-3.613	13.091	12.245	-3.143	-3.332
8	1855.71	0.640	-3.427	-3.613	13.079	12.237	-3.135	-3.324
9	1860.16	0.737	-3.426	-3.611	13.065	12.230	-3.125	-3.314

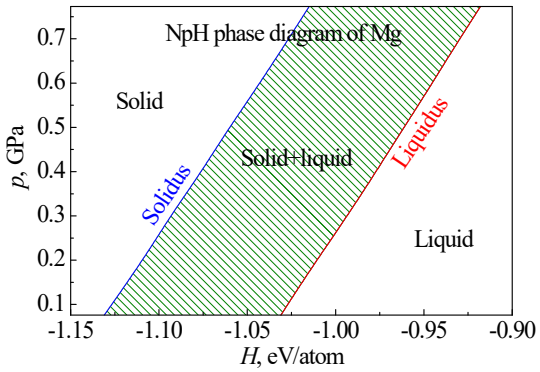
Mg

i	T K	p GPa	P_L eV/atom	P_S eV/atom	v_L Å^3/atom	v_S Å^3/atom	H_L eV/atom	H_S eV/atom
1	923.79	0.076	-1.163	-1.262	25.651	24.251	-1.031	-1.131
2	929.47	0.150	-1.163	-1.261	25.541	24.199	-1.019	-1.118
3	935.15	0.227	-1.163	-1.260	25.441	24.145	-1.006	-1.105
4	940.83	0.309	-1.163	-1.260	25.337	24.088	-0.992	-1.092
5	946.51	0.394	-1.163	-1.259	25.244	24.028	-0.978	-1.077
6	952.18	0.483	-1.163	-1.258	25.134	23.966	-0.964	-1.063
7	957.86	0.576	-1.163	-1.257	25.030	23.901	-0.949	-1.047
8	963.54	0.673	-1.163	-1.256	24.923	23.834	-0.934	-1.031
9	969.22	0.773	-1.163	-1.255	24.817	23.765	-0.918	-1.015

3. Finally, plot the lines of p-H_S and p-H_L to act as the solidus and liquidus so as to form the NpH phase diagram.







The rest data.

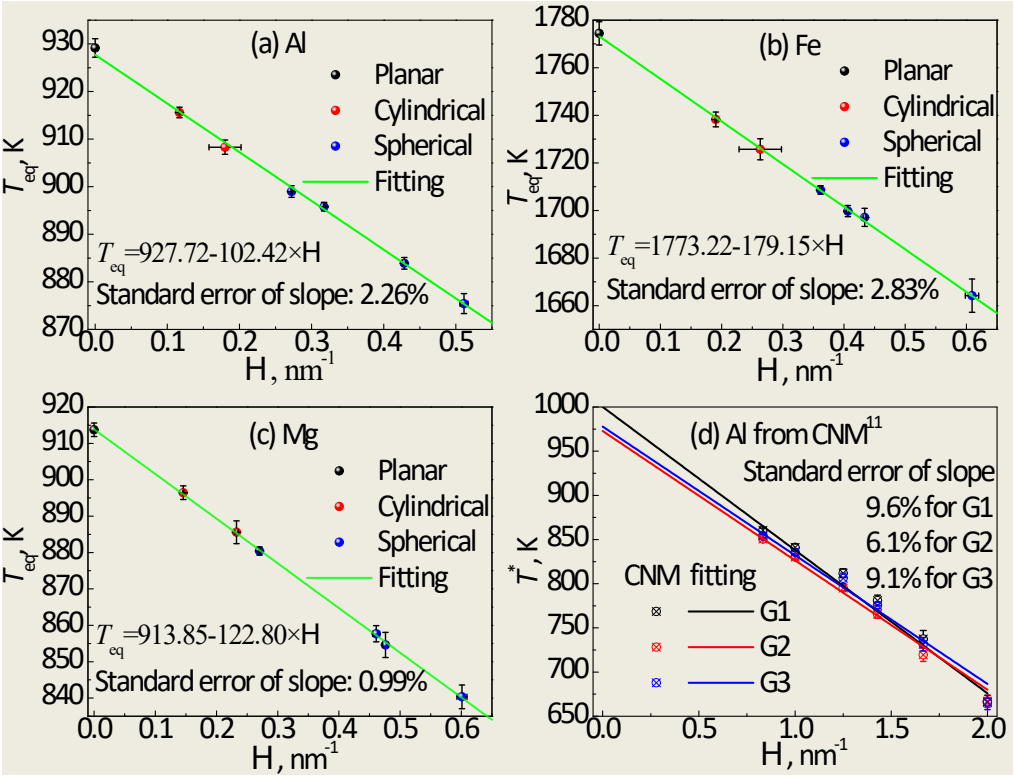


Table 1 The parameters required for the calculation of SL IFE according to SIM, the final results and the experimental and theoretical reference data.

Metal	T_m, K	ΔH_f, eV/atom	ΔS_f, eV/(atom·K)	Γ, K·nm	ρ_S, nm^{-3}
Al	929(2)	0.1119(15)	1.21(2)×10^{-4}	102(2)	56.41(11)
Fe	1777(4)	0.1871(26)	1.05(1)×10^{-4}	179(3)	80.23(6)
Mg	914(2)	0.1002(12)	1.09(1)×10^{-4}	123(1)	41.17(4)

Metal	γ_{SL}, mJ/m^2						
	This work	Exp. 1 *	Exp. 2	Model	CFM	CPM	CNM
Al	112(2)	93 [3]	163(21) [6]	155 [28]	149 [8]	-	163 [29]
Fe	241(4)	204 [3]	-	241 [28]	175(11) [9]	193.5(4) [27]	170 [30]
Mg	89(1)	-	-	100 [28]	89.9 [25]	-	-

* Exp. 1: maximum undercooling; Exp. 2: grain boundary groove method; Model: Turnbull model.